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Methanol Fueled Vehicles and Photochemical Models:

An Evaluation of the State of Knowledge

By

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Department of Environmental Sciences and Engineering
School of Public Health
University of North Carolina, Chapel Hill

May, 1989

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This study is part of the National Network for Environmental Management Studies conducted under the auspices of the Office of Cooperative Environmental Management -U. S. Environmental Protection Agency. This study is an evaluation of the ability of state-of-the-art photochemical mechanisms to assess the impacts of methanol fueled vehicles on ambient levels of ozone, formaldehyde and peroxyacetylnitrate (PAN). This evaluation involves comparing the predictions of the California Institute of Technology Mechanism (CIT), Carbon Bond Mechanism IV (CB4), and the Carter-Atkinson-Lurmann Mechanism (CAL) to observations from a series of smog chamber experiments previously conducted at the University of North Carolina. The evaluation demonstrates that the performance of the mechanisms decreases with increasing reactivity of the background mixture of ambient hydrocarbons.

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Abstract

This study is an evaluation of the ability of state-of-the-art photochemical mechanisms to assess the impacts of methanol fueled vehicles (MFVs) on ambient levels of ozone, formaldehyde, and peroxyacetylnitrate (PAN). This evaluation involved comparing the predictions of the California Institute of Technology Mechanism(CIT), Carbon Bond Mechanism IV (CB4), and the Carter-Atkinson-Lurmann Mechanism (CAL) to observations from a series of smog chamber experiments previously conducted at University of North Carolina.

The evaluation demonstrates that the performance of the mechanisms decreases with increasing reactivity of the background mixture of ambient hydrocarbons. For ambient mixtures characteristic of urban areas, CAL and CB4 would be expected to over estimate the absolute concentrations of ozone and PAN and under estimate the absolute concentrations of formaldehyde. The relative changes predicted by the mechanisms would be expected to under estimate the ozone control benefits of MFV programs. For more reactive hydrocarbon mixtures, CB4 and CAL performs better.

In this evaluation, CIT did not perform as well as CAL and CB4, particularly in the late afternoon and under conditions of low hydrocarbon and NO_x concentrations. It is difficult to generalize from these results, however, because the available documentation for the mechanism does not provide enough information to confirm its proper implementation.

A flow analysis of the formaldehyde chemistry of both CB4 and CAL determined that secondary production of formaldehyde accounts for 60 to 90% of all ambient formaldehyde. A large portion of this production is due to specific species such as ethylene.

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List of Abbreviations

Au	August
bhp-hr	brake horsepower-hour
CAL	Carter, Atkinson, Lurmann Mechanism
Cal Tech	California Institute of Technology
CARB	California Air Resources Board
CB4	Carbon Bond Mechanism-IX
CBM-III	Carbon Bond Mechanism-III
CEC	California Energy Commission
CIT	California Institute of Technology Mechanism
CMU	Carnegie-Mellon University
CO	carbon monoxide
DDA	General Motors-Detriot Diesel Allison
DNPH	dinitrophenylhydrazine
EKMA	empirical kinetic modeling approach
EPA	U.S. Environmental Protection Agency
ERT	Environmental Research and Technology, Inc.
FEP	fluorinated ethylene propylene
FFV	flexible fueled vehicle
FTP	federal test procedure
g	grams
GAO	U.S. General Accounting Office
HC	hydrocarbons
HCHO	formaldehyde
HNO_3	nitric acid
HONO	nitrous acid
HO_2	peroxyl radical
IR/MB	integrated rate/mass balance analysis
Jn	June
-K	with Killus's wall model
-M	with explicit representation of MeONO
MAN	Maschinefabrik Augsburg-Nurnberg
MeOH	methanol
MeONO	methyl nitrite
MFV	methanol fueled vehicle
mi	mile
min^{-1}	per minute
M85	85% methanol/15% gasoline
M100	100% methanol
-N	without a wall model
NAAQS	National Ambient Air Quality Standard
NO	nitrogen oxide
NO_x	nitrogen oxides
NO_2	nitrogen dioxide
PC-PKSS	Photochemical Kinetics Simulation System-personal computer version
ppm	parts per million
ppmV	parts per million by volume
OH	hydroxyl radical
OSHA	U.S. Occupational Safety and Health Administration
O_3	ozone

PAN	peroxyacetylnitrate
SAI	Systems Applications, Inc.
SAPRC	Statewide Air Pollution Research Center, University of California, Riverside
SCAQMD	South Coast Air Quality Management District
sec^{-1}	per second
St	September
SynAuto	synthetic automobile exhaust hydrocarbon mixture
SynAutoUrb	80% SynAuto/10% n-butane
SynUrban	synthetic urban hydrocarbon mixture
TSR	total solar radiation
TLV	threshold limit value
UNC	University of North Carolina, Chapel Hill
UTMA	U.S. Urban Mass Transportation Administration
UV	ultraviolet radiation

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Part I

An Overview

Ozone is a secondary air pollutant; it is not emitted into the air, but is produced in the atmosphere by chemical reactions of pollutants which are emitted into the air. The ambient concentration of ozone (O_3) is controlled by changing the emission levels of its precursors, namely nitrogen oxides (NO_x) and reactive hydrocarbons (HC). The same system of chemical reactions which produces ozone, however, also produces other secondary pollutants. A control measure designed to reduce ambient concentrations of ozone may simultaneously increase or decrease one or more of these other pollutants. Such side effects are especially important when they involve pollutants which are also hazardous or toxic, such as formaldehyde (HCHO).

The use of methanol fueled vehicles (MFVs) is an example of a control measure which may have such deleterious side effects. The combustion of methanol results in emissions of hydrocarbons which have less potential for producing ozone than those which result from burning gasoline or diesel fuel. While reducing ambient concentrations of ozone, there is concern that large-scale use of methanol may increase concentrations of formaldehyde, which is emitted directly from methanol combustion and is formed from unburned methanol (MeOH) by photochemical oxidation in the atmosphere.

To assess the air quality impacts of MFVs, or any other control measure, one must integrate information from a variety of different disciplines. This integration is presented schematically in Figure 1-1. The emissions of MFVs must be characterized and combined with information about current emissions and emission control programs to project what the mixture of future emissions will be. These projected future emissions, combined with projected meteorological conditions, can be used as inputs into a computer model of atmospheric processes. The model will predict the ambient concentrations of pollutants expected under the projected conditions. These predictions can be compared to what is known about the health effects of the pollutants to determine the effectiveness of the control measure.

The atmospheric models used in this process have two basic components: a chemical mechanism, which represents the chemical reactions of the pollutants; and a dispersion mechanism, which represents the dispersion, diffusion, and transport of the pollutants. The chemical mechanisms that are currently used have been almost exclusively designed to predict peak ozone concentrations given pollutant mixtures which are common to urban areas, and they do this quite well (within 30%). It is not clear, however, if the models are capable of predicting concentrations of other pollutants or

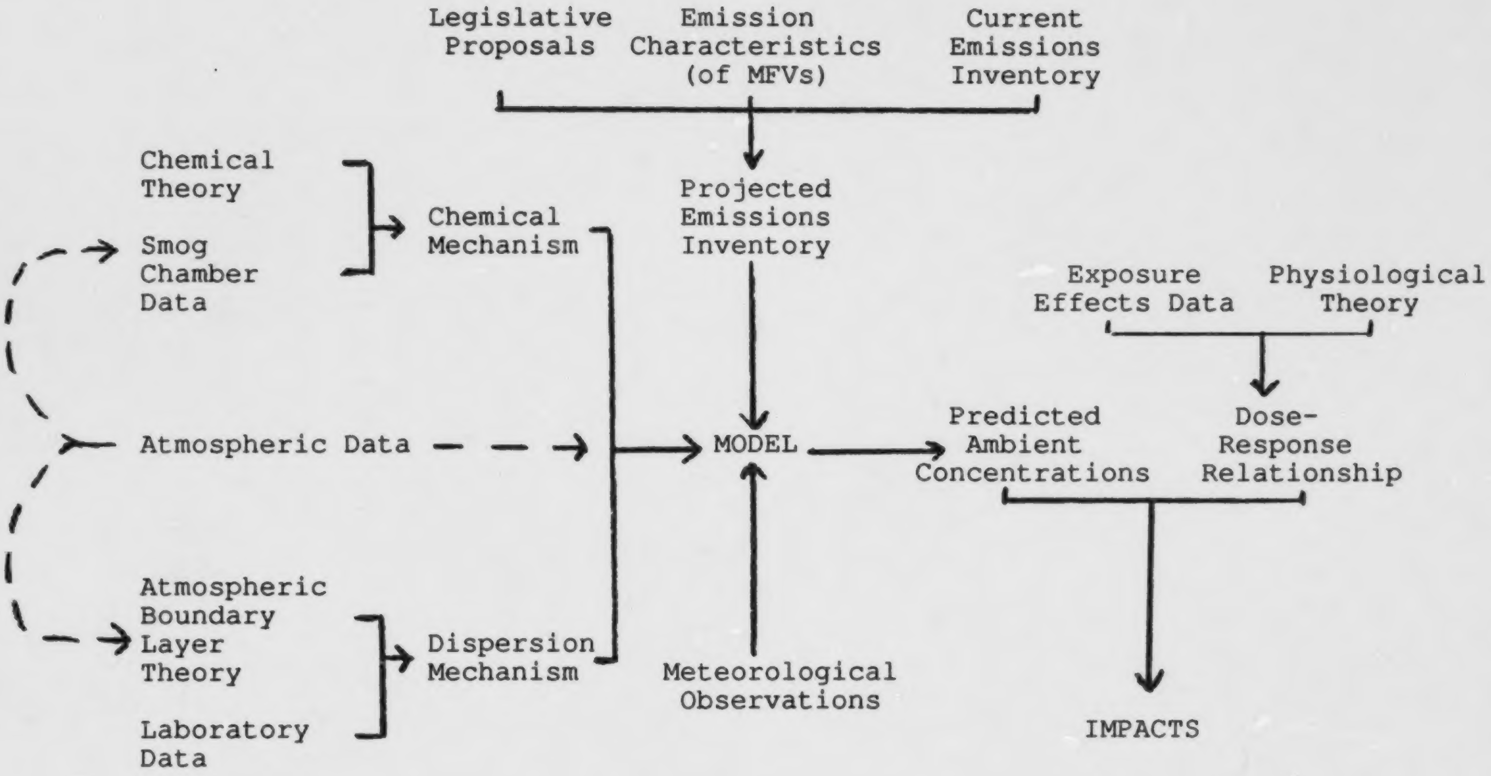

Legislative Proposals
Emission Characteristics (of MFVs)
Current Emissions Inventory
Chemical Theory
Smog Chamber Data
Chemical Mechanism
Projected Emissions Inventory
Exposure Effects Data
Physiological Theory
Atmospheric Data
MODEL
Predicted Ambient Concentrations
Dose-Response Relationship
Atmospheric Boundary Layer Theory
Laboratory Data
Dispersion Mechanism
Meteorological Observations
IMPACTS

FIGURE 1-1: The Structure of An Impact Assessment for Methanol Fueled Vehicles

of predicting ozone concentrations given a very different mixture of emissions.

My primary purpose in this study is to evaluate the ability of state-of-the-art photochemical mechanisms to assess the impacts of MFVs on ambient levels of ozone, formaldehyde, and peroxyacetylnitrate (PAN). This evaluation involves comparing the predictions of several current mechanisms to observations from a series of smog chamber experiments.

As part of this evaluation, I must assess whether the pollutant mixtures used in the chamber experiments are representative of the type of methanol fueled vehicles, the amount of usage, and the composition of exhaust emissions that would be expected from the use of MFVs. I must also define the specific types of air quality impacts that I am interested in predicting for each of the three pollutants. I discuss these concerns, the philosophy of model development and testing, and the conclusions of past MFV modeling assessments in Part 1 of this report.

In Part 2 of this report, I present the actual comparison of mechanism predictions and chamber observations. Based on the findings of this comparison, I evaluate the utility of the mechanisms in addressing the impacts of MFVs, the control of ambient HCHO levels, and other future air quality concerns.

Three appendices accompany this report: Appendix A contains an experiment-by-experiment description of the mechanism evaluation; and Appendices B and C contain computer file listings of the initial conditions and photolytic rates which would be needed to verify or replicate the evaluation.

mechanism evaluation; and Appendices B and C contain computer file listings of the initial conditions and photolytic rates which would be needed to verify or replicate the evaluation.

Methanol Fuel Technology

Reasons for Interest

Methanol has received serious consideration as an alternative fuel for motor vehicles since the energy crisis of the late 1970s when it was seen as a way to reduce this country's dependence on foreign oil [California Energy Commission (CEC), 1986]. While methanol is currently produced from natural gas and residual oil, it can be produced from such plentiful domestic resources as wood, agricultural waste, and municipal waste. The most likely domestic feedstock for methanol production, however, is coal. Currently there are no coal-to-methanol facilities in the United States, but several processes of coal gasification and subsequent methanol synthesis are commercially possible [Environmental Protection Agency (EPA), 1982].

In recent years, methanol has received attention as an alternative to gasoline and diesel fuels because of its potential benefits to air quality. In urban areas, gasoline and diesel fueled vehicles are responsible for 30 to 50% of the hydrocarbon precursors of ozone and 80 to 90% of the carbon monoxide emissions [EPA, 1987a]. In some areas, diesel fueled vehicles are responsible for as much as 50% of the ambient particulate matter [General Accounting Office (GAO), 1986]. Motor vehicles also contribute heavily to levels of toxic air contaminants and are estimated to be responsible for 90% of the benzene present in the atmosphere [California Air Resources Board (CARB), 1986].

Because of methanol's simple molecular structure, methanol combustion results in hydrocarbon emissions which may produce less ozone than the emissions from gasoline or diesel vehicles. Methanol has a high octane rating, low flame temperature, and wide flammability limits which create the potential for MFVs to be designed to produce less NO_x or carbon monoxide (CO) than conventionally fueled vehicles [EPA, 1987a]. MFV emissions also contain less particulate matter and no heavy organics [GAO, 1986].

MFVs are similar to conventionally fueled vehicles in performance and driveability. On a volume basis, methanol has about half the energy content of gasoline. In other words, it takes 2 gallons of methanol to travel as far as one can on 1 gallon of gasoline. Currently, the price of methanol fuel is about half that of gasoline, and therefore, methanol is equivalent to gasoline in terms of miles travelled per dollar [CEC, 1986].

Vehicle and Engine Types

The engines of current light-duty MFVs are actually gasoline engines which have been modified to make them compatible with methanol fuels. Metals such as lead, tin, zinc, and aluminum will corrode when exposed to methanol, so fuel lines and tanks must be made of stainless steel. Many of the seals and gaskets used in gasoline engines must also be replaced with other materials to avoid deterioration. Because of methanol's low surface ignition temperature, the spark plugs and ignition timing must be modified [GAO, 1986]. Because methanol emissions do not contain any lead or sulfur compounds which poison catalysts, catalytic converters may be made with base metals, such as copper or chromium, instead of expensive noble metals, such as platinum and palladium [EPA, 1982]. The durability of current MFV engines has not been determined, and engineers are continuing to test alternative materials and motor oil formulations [GAO, 1986].

These current MFVs use a fuel mixture of 85% methanol and 15% gasoline, designated as M85. The gasoline is added to improve the volatility of the fuel under cold start conditions because pure methanol will not vaporize enough to form a flammable mixture at temperatures below 50°F. Cold starting is also improved by the addition of a carburetor heater which heats the fuel mixture before it is injected into the combustion chamber [GAO, 1986].

Gasoline is also added to the methanol fuel for several safety reasons: it increases the luminosity of the methanol flame making it easier to see in the event of an accidental fire, and it acts as a taste deterrent to discourage human consumption of the fuel. However, adding gasoline also increases the flammability of the fuel and the chance of explosion [Fanick et al., 1984].

In the future, it is expected that MFVs will be designed specifically to run on pure methanol, designated as M100. Utilizing advanced fuel injection, high compression, and lean combustion, advanced MFVs could fully capitalize on the reduced emissions of methanol combustion. Formaldehyde emissions could be virtually eliminated using an emission control catalyst specifically designed for MFVs [EPA, 1987a]. Toyota Motor Corporation has developed a lean combustion engine which runs cleaner on M100 than current MFVs, but they have yet to overcome the cold start problem with pure methanol [Murrell and Piotrowski, 1987].

MFVs with modified gasoline engines could feasibly be mass produced by 1995. Advanced MFVs would be expected to follow within approximately five years. To bridge the gap between gasoline and methanol, Ford Motor Company has developed a flexible fueled vehicle (FFV) which runs on methanol, gasoline, or any mixture of the two. An on-board computer adjusts the FFV's engine using an optical sensor which characterizes the fuel mixture and other sensors which measure the air flow into the engine and the oxygen content of the exhaust [GAO, 1986]. Most likely, FFVs will operate on a fuel mixture of approximately 35% methanol and 65% gasoline [CARB, 1989].

The development of heavy-duty MFVs, trucks and buses, is not as advanced as for light-duty MFVs. Prototype methanol buses have demonstrated driveability and performance similar to diesel buses and much lower emissions of NO_x and particulate matter, but further research is needed to determine the durability of the methanol engines and to optimize the design of emission control systems [CEC, 1986].

Current Programs and Proposals

While federal legislation promoting alternative fuels remains pending, the State of California leads the nation in the move to methanol fuels. Currently, over 500 light-duty MFVs are operated throughout California by state agencies and two private firms [CEC, 1986]. The California Energy Commission (CEC) has recently entered into agreements with two gasoline distributors, ARCO and Chevron, to establish a network of methanol pumps throughout the state [McNary, 1988]. The South Coast Air Quality Management District (SCAQMD), which oversees the Los Angeles area, passed a rule last year which requires gasoline service station owners to install methanol compatible underground storage tanks when they replace old tanks. This year the district is considering a rule which requires operators of all public or private fleets consisting of 15 or more vehicles to purchase only vehicles which operate on an alternative fuel. FFVs are seen as the most likely vehicles to fill this requirement [SCAQMD, 1988]. By the year 2000, SCAQMD would like to see more than 1 million MFVs on the road out of the expected 8 million vehicles in the Los Angeles area [McNary, 1988]. Promoting the use of methanol fuels in stationary sources, the district has proposed a three-year phase out of the use of fuel oils and solid fossil fuels in stationary sources beginning in 1992 [SCAQMD, 1988].

In 1983, California began the first methanol bus demonstration program in the United States. Since then the Golden Gate Transit District in San Rafael, California, has been operating a methanol bus manufactured by General Motors-Detroit Diesel Allison (DDA) and one manufactured by Maschinenfabrik Augsburg-Nurnberg (MAN) of West Germany. With funding from the Urban Mass Transportation Administration (UMTA), Florida's Department of Transportation has developed a retrofit procedure to convert diesel buses to methanol using technology similar to that used in the DDA bus. Other methanol bus programs have been implemented or considered for Los Angeles, California; Riverside, California; Seattle, Washington; New York, New York; Denver, Colorado; Madison, Wisconsin; Lowell, Massachusetts; and Charleston, West Virginia [GAO, 1986].

Composition of Emissions

Present emission standards for gasoline fueled vehicles apply to exhaust hydrocarbons, carbon monoxide, nitrogen oxides, evaporative hydrocarbons, and crankcase emissions. Emission standards for diesel fueled vehicles presently apply to exhaust hydrocarbons, carbon monoxide, nitrogen oxides, crankcase emissions, particulate matter, and smoke.

So as not to put methanol fuels at a competitive disadvantage, the U.S. Environmental Protection Agency (EPA) has promulgated emission standards for MFVs which would be equivalent to the present standards for conventionally fueled vehicles [EPA, 1986]. Under EPA's new regulations, MFVs would assume the same emission standards for carbon monoxide, nitrogen oxides, particulate matter, and smoke as the light-duty or heavy-duty conventional vehicles that they replace. The emission standards for exhaust and evaporative hydrocarbon emissions, however, are not as easily substituted between fuel types. Organic emissions from gasoline engines are almost entirely composed of non-oxygenated hydrocarbons which react with nitrogen oxides to produce ozone. Emissions from MFVs, on the other hand, contain large quantities of the oxygenated hydrocarbons methanol and formaldehyde. While methanol is less photochemically reactive than most of the non-oxygenated hydrocarbons emitted from gasoline fueled vehicles, formaldehyde is more reactive than most of the gasoline emissions. Taking into account these differences in ozone producing potential, EPA has made the hydrocarbon emission standards for MFVs and gasoline fueled vehicles equivalent on the basis of the amount of organic carbon emitted. The standard is implemented by converting measured amounts of methanol and formaldehyde into equivalent amounts of non-oxygenated hydrocarbons based on empirically measured molecular weights.

The MFV emission standards for CO and NO_x are the same as those for gasoline fueled vehicles. While reductions in these pollutants may be possible in the future, the technology to reduce CO is not yet available, and EPA believes that manufacturers will tradeoff possible NO_x reductions for greater performance and fuel economy [EPA, 1987a].

Gold and Moulis [1987] compiled emission measurements of MFVs from 13 different studies. Out of the vehicles tested in these studies, 40 MFVs met the Federal Test Procedure (FTP) emission standards for CO and NO_x. Only one of the studies, the Alcohol Fueled Test Program of the California Air Resources Board, included adequate measurements of non-oxygenated hydrocarbons. Of the six vehicles in the CARB study, three were fueled with M85, two with M88, and one with M90. Based on the relative proportions of methanol, formaldehyde, and non-oxygenated hydrocarbons in the exhaust of these vehicles, Gold and Moulis [1987] projected the composition of methanol exhaust required to meet the MFV carbon-based standard. These maximum hydrocarbon emission levels are shown in Table 1-1 along with the maximum emission levels for CO and NO_x. Table 1-1 also includes the average and range of emissions of the 40 MFVs which met the CO and NO_x emission standards. It is interesting that while gasoline comprised a maximum of 15% of the fuel mixture gasoline related emissions comprised almost 40% of the exhaust.

Emissions of a new car tuned to the manufacturer's specifications that are designed to meet the FTP standards may differ considerably from the actual in-use emissions of vehicles driven by the general public. Snow et al. [1989] recently characterized the emissions from an in-use M85-fueled vehicle under non-certification conditions. The results of this study are shown in Table 1-2. For comparison the composition of emissions of a typical gasoline fueled vehicle, assuming identical organic emission rates, is shown in parentheses. The composition of these in-use MFV emissions is very close to the composition proposed by Gold and Moulis [1987].

In several studies of MFV emissions, quantities of methyl nitrite (MeONO) have been measured [Smith and Urban, 1982]. It is formed, not in the combustion chamber, but in the exhaust by reaction of methanol with nitrogen dioxide (NO_2). Because measurable quantities have only been formed at low dilution ratios, it is not clear how much methyl nitrite is actually formed or if the formation is merely an artifact of the measurement process. In their review of methanol photochemistry, Ballentine et al. [1985] observed that the only fate of methyl nitrite is photodissociation into formaldehyde and radicals, and therfore, it may be important to the formation of ozone. The importance of possible methyl nitrite emissions is discussed further in Part 2 of this report.

TABLE 1-1: FTP Emission Factors for Current MFVs

Pollutant	Proposed Standard	Average Emissions	Range
Methanol	0.546 (g/mi)	0.47	0.12-1.00
Formaldehyde	0.048	0.035	0-0.17
Non-Oxygenated HC	0.152	?	?
CO	3.4	1.7	0.43-3.2
NOx	1.0	0.61	0.04-0.88

Source: Gold and Moulis [1987]

TABLE 1-2: In-Use Hydrocarbon Emissions from a Current MFV (and a typical gasoline fueled vehicle)

Pollutant	Tailpipe (g/mi)	Evaporative (g/mi)	Refueling (g/mi)	Total (g/mi)	% of HC
Methanol	0.96 (0.00)	0.31 (0.00)	0.05 (0.00)	1.32 (0.00)	58.7
Formaldehyde	0.12 (0.01)	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)	5.3
Non-Methane HC	0.33 (1.35)	0.17 (0.48)	0.15 (0.20)	0.65 (2.03)	28.9
Methane	0.16 (0.21)	0.00 (0.00)	0.00 (0.00)	0.16 (0.00)	7.1
Total	1.57 (1.57)	0.48 (0.48)	0.2 (0.20)	2.25 (2.25)	100.0

Values in parentheses are for a typical gasoline vehicle.
Source: Snow et al. [1989]

While the design of heavy-duty methanol engines is still in the early stages of development, initial emission measurements of methanol buses show considerable advantages over their diesel counterparts. Table 1-3 shows the emissions of the two buses included in Golden Gate Transit District's demonstration program that was described earlier and the average emissions from three new diesel bus engines. Further development of heavy duty engines and emission control systems should lead to great reductions in CO, NOx, particulate matter, as well as hydrocarbons [GAO, 1986].

Recently, CARB has promulgated its own emission standards for MFVs [CARB, 1989]. In addition to setting the emission levels of organic carbon, NO_x, and CO to the same levels as required for conventionally fueled vehicles, CARB established a formaldehyde emission standard to assure that MFVs will not exceed the upper limits of formaldehyde emissions from conventionally fueled vehicles. The level has been set at 15 mg/mi for light duty MFVs and at 0.1 g/bhp-hr for heavy duty MFVs. Several intermediate levels apply to vehicles of intermediate weight. The standards are going to be phased in over the years 1993 to 1995 during which less stringent standards will be applied.

TABLE 1-3: A Comparison of Emissions from Diesel and Methanol Bus Engines Over Various Test Cycles

Pollutant	Diesel Engine (g/bhp-hr)	MAN Engine (g/bhp-hr)	DDA Engine (g/bhp-hr)
Particulate Matter	0.57	0.04	0.17
NO_x	6.25	6.60	2.20
CO	3.22	0.31	1.31
Non-Oxygenated HC	1.51	0.001	0.0
Methanol	0.0	0.68	1.13
Aldehydes	0.10	0.001	0.15
Test Cycle	EPA transient	EPA transient	13-mode steady-state

Source: EPA [1986]

Measures of Air Quality Impacts

While the potential exists for MFVs to have a wide variety of air quality benefits in the future, current technology and regulations focus on the difference in the composition of hydrocarbons emitted by MFVs as compared to conventionally fueled vehicles. The composition of the hydrocarbon emissions from MFVs is expected to reduce the formation of secondary pollutants, such as ozone and PAN. At the same time, there is concern that MFVs will increase the ambient levels of formaldehyde both through direct emissions and secondary formation from unburned methanol.

To assess the impact of MFVs, one must understand how each of these pollutants impacts human health and welfare and define some measure of this impact. If the primary effect of a pollutant is an acute respiratory response, then a daily maximum concentration may be an appropriate measure of the impact. A peak concentration, however, would not be an adequate measure of a chronic impact such as human cancer or materials damage. It is changes in these measures of impact that one must predict in assessing MFVs. In this section, I define measures of impact for ozone, formaldehyde, and PAN that will serve as performance criteria for the mechanism evaluation in Part 2.

Ozone

The current National Ambient Air Quality Standard (NAAQS) for ozone is a one-hour maximum concentration of

0.12 ppm which is not to be exceeded more than once per year on the average over a three year period. Persons subject to concentrations above this level have experienced a variety of respiratory and non-respiratory symptoms including throat dryness, chest tightness, cough, pain on deep inspiration of breath, fatigue, headache, and nausea. Acute exposure to ozone can modify pulmonary function as quantitatively measured by, but not limited to, forced expiratory volume (FEV), tidal volume, and breathing frequency. A recent review of the NAAQS standard for ozone conducted by the EPA concluded that there is no clear evidence that individuals with existing respiratory diseases are affected more by ozone exposure than healthy individuals. Exposure to ozone, however, may impair the mucociliary, phagocytic, and immunological defenses of the repiratory system [EPA, 1987b].

Animal toxicology studies of several species have shown consistent morphological damage despite differences in lung structure between the species. There is also some evidence from animal studies that recovery of normal pulmonary function after chronic exposure to ozone does not occur even after an extended period of time [EPA, 1987b]. An epidemiological study of children exposed to a smog episode in which one-hour peaks ranged between 0.135 and 0.186 ppm ozone showed that lung function decrements can persist for as long as a week [Lioy et al., 1985]. Despite this evidence, the EPA review concluded that "little is known with certainty regarding either long-term implications of repeated acute ozone exposures or chronic effects of prolonged exposure of humans to ozone [EPA, 1987b]."

Exposure to ozone also causes damage to materials such as rubbers, elastomers, and paints. In fact, in the 1950's the ambient concentration of oxidants was measured by the time for cracking to appear in a piece of rubber exposed to the ambient air [Finlayson-Pitts and Pitts, 1986]. The discovery of photochemical smog itself was based on studies of injury to plants in the Los Angeles basin. Today, ozone continues to be a major cause of crop damage in the state of California. EPA is currently considering promulgating a secondary ozone standard designed to reduce plant and materials damage.

Currently, not enough is known about chronic health effects and plant and materials damage due to ozone exposure to evaluate the importance of such impacts. Given that 60 urban areas around the country have not yet met the primary ambient standard, however, the focus of ozone control efforts remains on the acute respiratory response to peak concentrations. Thus, I define the ability to predict peak ozone concentrations as an appropriate performance criterion for the mechanism evaluation.

Formaldehyde

Formaldehyde is a pungent gas with an odor threshold of approxiamately 1 ppm. While the threshold limit value (TLV) is defined by the American Conference of Government Industrial Hygienists to be 1 ppm, exposure to concentrations as low as 0.1 ppm can cause irritation of the eyes, nose, and throat. Human volunteers exposed to a concentration of 0.3 ppm for 4 to 5 hours have shown inhibited nasal mucociliary function. Pneumonia, bronchial inflammation, and pulmonary edema have been caused by exposures to concentrations greater than 50 ppm, and exposure to a concentration of 100 ppm is defined by the Occupational Safety and Health Administration (OSHA) as "immediately dangerous to life and health [OSHA, 1987]." Currently, there is not a NAAQS for formaldehyde.

In proposing emission standards for MFVs, EPA evaluated several human exposure scenarios which they felt had the greatest potential for causing significant acute health effects [EPA, 1986]. These scenarios included exposure in street canyons, tunnels, expressways, public parking garages, and personal garages. Recognizing the difficulty in establishing a clear threshold for irritant effects, especially among the most sensitive populations, EPA chose to use an ambient formaldehyde concentration of 0.40 ppm as "a reasonable level of concern [EPA, 1986]." The street canyon, tunnel, and expressway scenarios resulted in ambient concentrations of methanol and formaldehyde which pose no significant risk to public health even under the assumption that 100% of the vehicle fleet consisted of MFVs with exhausts comprised of 8% formaldehyde. The public garage scenario produced levels of formaldehyde which approached levels of concern when several worst-case conditions occured simultaneously. This simultaneous occurence was considered unlikely. The personal garage scenario resulted in ambient levels of formaldehyde at twice the level of concern when the emissions control devices were disconnected or malfunctioning. Given the minor health effects which would occur from such exposure and the individual's responsibility to maintain the vehicle, EPA found no basis for regulating formaldehyde emissions based on this scenario. Thus, EPA determined that the standards based on the total organic emissions were adequate to protect human health from the acute toxicological effects of emissions from MFVs [EPA, 1986].

EPA and the International Agency for Research on Cancer have classified formaldehyde as a probable human carcinogen [EPA, 1986]. Epidemiological evidence of human carcinogenicity is limited, but two animal studies have definitively shown that formaldehyde can produce nasal cancer in rats and mice. One of these studies, conducted by the Chemical Industry Institute of Toxicology, is the basis of carcinogenic risk estimates by both EPA and OSHA. The upper 95% confidence levels for individual lifetime cancer risk due to exposure to 1 ppm as estimated by these agencies are 1.9 x 10^{-6} and 2.6 x 10^{-3}, respectively [Carey, 1987; OSHA, 1987]. While more research is needed to define the carcinogenic mechanism and dose-response relationship, some animal bioassays suggest that the intensity of the formaldehyde exposure may be more important than the duration of the exposure for the carcinogenic process [Nelson et al., 1986].

In their proposed MFV emission standards, EPA recognized that "an increase in mobile source emissions of formaldehyde would tend to increase average ambient levels as well as any attendant cancer risk [EPA, 1986]." However, due to the uncertainty concerning the impact of MFVs on ambient concentrations of formaldehyde as well as the potency of formaldehyde as a human carcinogen, EPA decided not to propose any emissions standard based on carcinogenicity.

Based on the EPA assessment, there does not appear to be a threat of acute effects from ambient levels of formaldehyde except in severe situations. Because cancer risk is a concern, though, it is important to evaluate the integrated exposure as well as the maximum concentration. Thus, instead of using the ability to predict peak concentrations as a mechanism performance criterion, I will evaluate the mechanisms' ablities to duplicate the entire formaldehyde concentration profile.

PAN

PAN, or peroxyacetylnitrate, is one of the predominant forms of oxidized nitrogen in ambient air. Along with aldehydes, this explosive gas is considered to be responsible for the eye irritation associated with photochemical smog. There is no specific NAAQS for PAN and significant adverse health effects have only been observed at high concentrations [EPA, 1987b]. Because of its acute effects, I choose the ability to predict peak concentrations of PAN as a performance criterion for the mechanism evaluation.

Photochemical Modeling

The Purpose of Models

To assess the impacts of air quality control strategies, one must establish a quantitative relationship between emissions and ambient concentrations of pollutants. Ambient concentrations, however, are affected by many processes other than emissions, including meteorology, topography, chemical reactions, physical transformations, and deposition processes. Air quality simulation models are designed to mathematically represent these processes and predict ambient concentrations over space and time as functions of the emissions distribution, meteorology, and topography.

Seinfeld [1988] distinguished between air quality models that are prognostic, or based on fundamental physical and chemical principles, and models which are diagnostic, or based on statistical descriptions of observed air quality. The models discussed in this report are prognostic. Seinfeld [1988] also defines four structural levels of a model:

(1) a set of assumptions and approximations that reduce the actual physical problem to an idealized one that retains the most important features of the actual problem;

(2) the basic mathematical relations and auxiliary conditions that describe the idealized physical system;

(3) the computational schemes that are used to solve the basic equations; and

(4) the computer program or code that actually performs the calculations.

In this report, the term "model" refers to all of these levels.

Modeling Primary vs. Secondary Pollutants

The modeling of primary pollutants, those which are directly emitted into the atmosphere (eg. CO, sulfur dioxide, and particulate matter), is typically accomplished with Gaussian plume models. These models approximate the dispersion and diffusion of an emission plume as a normal distribution of concentrations in both the crosswind and vertical directions. Given meteorological conditions and source characteristics, the concentration resulting from a single source is calculated for a particular point in space and time. Typically, the contributions of multiple sources are each calculated separately and then added together. Gaussian equations require simple computations but do not represent spatial and temporal variability well. These models also are not adequate to predict concentrations of secondary pollutants which are formed in the atmosphere by reactions of primary pollutants. [Finlayson-Pitts and Pitts, 1986]

The modeling of reactive or secondary pollutants (eg. O_3, HCHO, and PAN) is accomplished using numerical models based on the conservation of mass as expressed by the atmospheric diffusion equation, or K-theory [Dobbins, 1979]. As explained in the initial overview, these models are basically composed of two submodels: a dispersion mechanism and a chemical mechanism. The dispersion mechanism describes the atmospheric transport and diffusion of pollutants based on emissions, meteorology, and topography. The chemical mechanism is actually a set of chemical reactions and their rates which may be converted into a system of coupled differential equations. This system of reactions is solved simultaneously with the dispersion mechanism to yield concentrations as functions of time and space. The formulations of these models are typically based on two forms of the atmospheric diffusion equation: the Lagrangian and the Eulerian.

Lagrangian, or trajectory, models focus on one parcel or column of air. As winds carry this parcel of air over a given trajectory, it is subject to pollutant inputs, dilution, and chemical reaction [Finlayson-Pitts and Pitts, 1986]. Lagrangian models do not account for horizontal diffusion across the boundaries of the parcel, the vertical component of the wind, and variation in wind speed and direction with height [Liu and Seinfeld, 1975]. These models have the advantage, however, of being less computationally expensive, requiring less input data, and allowing easier modification of the chemical mechanism than Eulerian models. The Empirical Kinetic Modeling Approach (EKMA) model, which is recommended by EPA for calculating the ozone control requirement for most areas, is a simple trajectory model of this type [Hogo and Gery, 1988].

Eulerian, or grid-based, models represent an airshed as a three dimensional array of cells. By accounting for chemical reactions within each cell and flows into and out of each cell, pollutant concentrations are calculated for each cell over time. The error introduced by the finite differencing assumptions used to solve the differential equations in these models decreases as the grid resolution increases [Johnson et al., 1976]. However, the maximum resolution achievable under the fundamental assumptions of the atmospheric diffusion equation are cell areas of 2 km^2, cell heights of 20 m, and time intervals of 15 minutes [Lamb and Seinfeld, 1973]. The ability to evaluate air quality control strategies on a geographical basis is a major advantage of Eulerian models, but they have extensive data input requirements and are expensive to run [Finlayson-Pitts and Pitts, 1986].

Model Evaluation

Evaluating the accuracy of model predictions is an inherently difficult process. Both Lagrangian and Eulerian models predict ambient concentrations as averages over areas of several square kilometers and time intervals of about an hour. These averages are not necessarily comparable to ambient monitoring data gathered at fixed points. Thus, no definitive measure of model performance exists [Seinfeld, 1988]. Furthermore, it is difficult to reconstruct definitively the meteorological conditions and emissions information with the appropriate level of spatial and temporal resolution for a given day [Schere, 1988]. The extensive input conditions, the formulation of the dispersion mechanism, the formulation of the chemical mechanism, the computational schemes, and the computer codes are all sources of uncertainty that could contribute to error in the model predictions. Even if a model is able to produce predictions similar to those observed on given day, the agreement may be due to compensating errors. Thus, the question often asked by modelers, "Are we getting the right answers for the right reasons?" Unfortunately, one can never answer this question affirmatively with complete confidence. Model evaluation is an inductive process: one can never prove that a model is correct, one can only show that it is not wrong.

Errors in the formulation of the model can be evaluated by isolating the components of the model and testing them against simplified systems in which there are, theoretically, fewer sources of uncertainty. Independent of chemical reactions and continuous emissions, predictions of the dispersion mechanism may be compared to analytical flow representations that have exact solutions and to observations in atmospheric tracer studies [Schere, 1988]. Independent of transport and diffusion, predictions of the chemical mechanism may be compared to observations in smog chamber studies. It is this sort of chemical mechanism evaluation that is the focus of this report.

Smog Chamber Studies

The primary purpose of smog chamber studies is to provide data for the development and evaluation of chemical mechanisms, not to simulate pollutant behavior in the atmosphere. Besides the absence of continuous emissions and complex meteorology, smog chambers differ from the ambient atmosphere in several important ways. The surface area created by the walls of the chamber is the single largest source of uncertainty in using the chamber as a surrogate for the ambient atmosphere. While there are surfaces present in the urban atmosphere created by particulate matter, the surface to volume ratio is much lower than in a chamber. Changes in gas phase concentrations of several species that cannot be explained on the basis of known homogenous gas phase reactions have been observed in most chamber experiments. These changes have been attributed to unknown heterogeneous reactions occuring on the walls and the outgassing of vapors deposited on the wall from previous experiments. These wall effects vary considerably depending on chamber characteristics, chamber history, light intensity, temperature, relative humidity, and initial pollutant concentrations [Finlayson-Pitts and Pitts, 1986].

Another major source of uncertainty in using the chamber as a surrogate for the ambient atmosphere is the light characteristics of the chamber. The spectrum of light inside the chamber is dependent on the source of light, whether it be a xenon lamp or the natural sun, and the light transmission properties of the chamber walls, which are typically made of Teflon [Finlayson-Pitts and Pitts, 1986].

Despite differences with the ambient atmosphere, smog chamber experiments provide an opportunity to observe the complex, non-linear system of photochemical reactions under controlled conditions. Characteristic time-concentration profiles for several pollutants, which would be seen in both chamber experiments and urban atmospheres, are shown in Figure 1-2. In the early morning hours, nitric oxide (NO) and HC concentrations are high due to injection into the chamber or emissions into the atmosphere. As the sun rises and begins to act on the mixture of pollutants, NO is converted to NO_2 through a process initiated by hydroxyl radical (OH) attack on hydrocarbons. When NO concentrations reach relatively low levels, O_3 begins to accumulate. In the afternoon when NO and HC concentrations are low, free radicals oxidize NO_2 yielding PAN, nitric acid (HNO_3), and lesser amounts of particulate nitrate. HCHO concentrations increase throughout the beginning of the day as it is formed

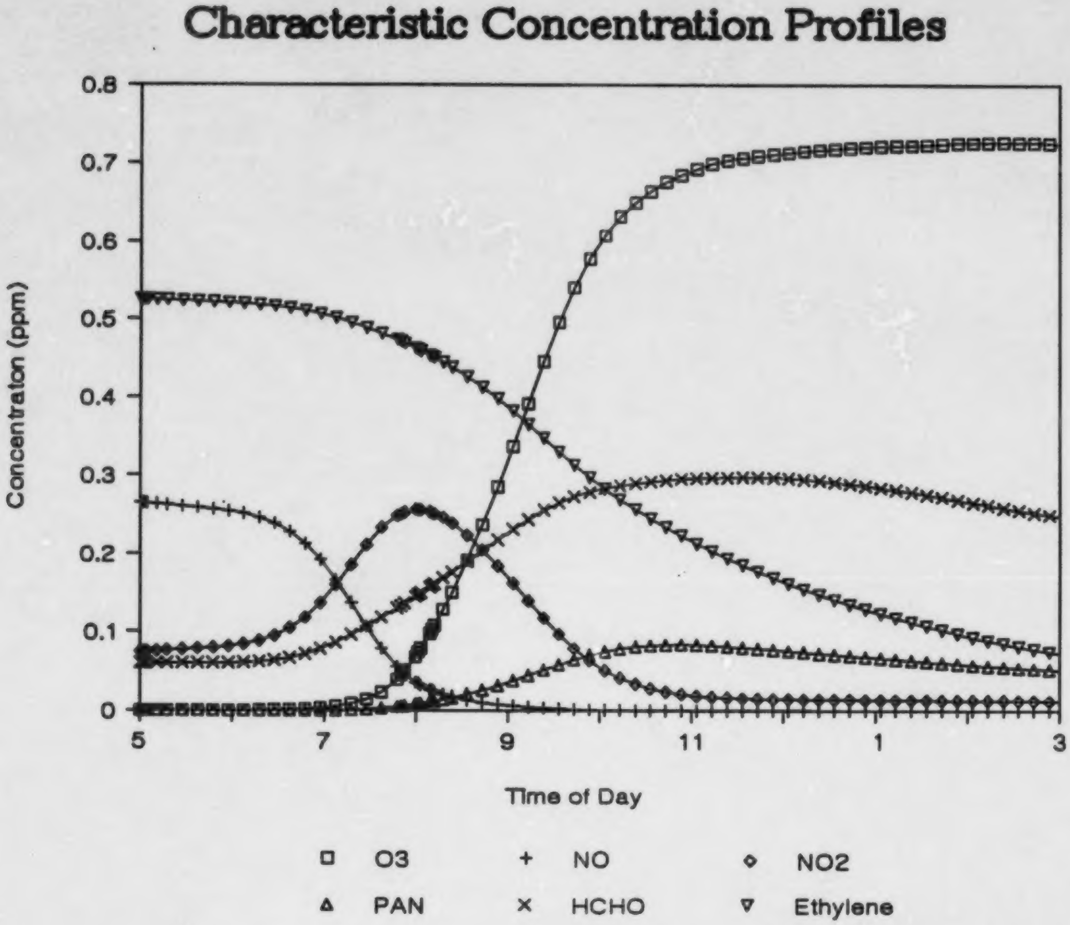


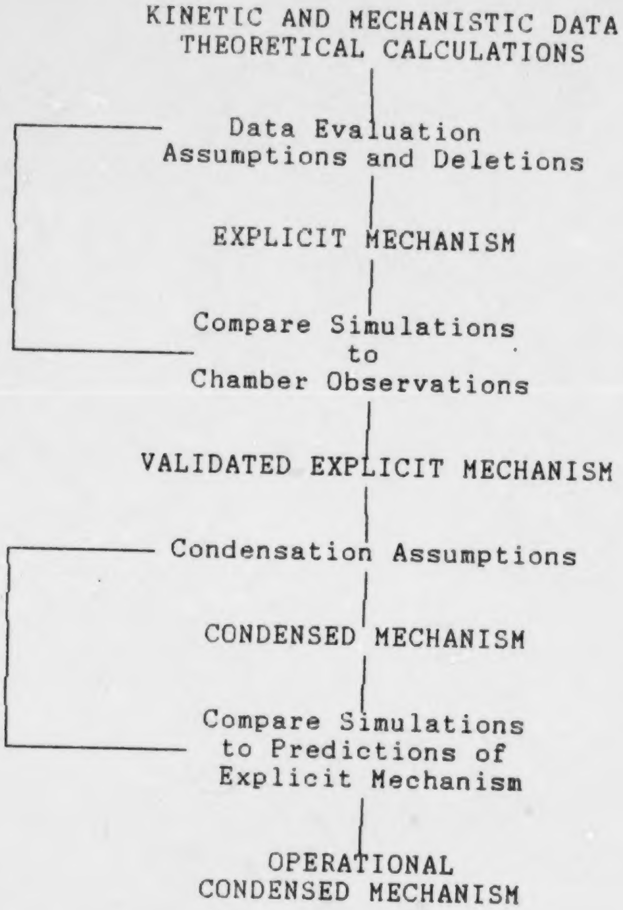
Figure 1-2. Characteristic Concentraton Profiles

by the decomposition of more complex hydrocarbons. In the afternoon, HCHO is consumed by OH attack and photodissociation. [Finlayson-Pitts and Pitts, 1986]

Development of the Chemical Mechanism

Regardless of their complexity, the chemical mechanisms used in air quality simulation models are simplified representations of the complex photochemistry which occurs in the real world. Models are created from real world observations through the processes of generalization, deletion, and distortion [Jeffries and Arnold, 1987b]. The usefulness of a model depends on the completeness and goodness of its generalizations [Jeffries, 1988d]. Modelers test their generalizations, deletions, and distortions one at a time in an iterative process of model development and evaluation, summarized in Figure 1-3. From empirical determinations of reaction pathways and rates, modelers list all the important reactions which are known to occur. Given uncertain or unknown reaction rates or pathways, modelers make assumptions based on theoretical calculations. The resulting detailed, or explicit, mechanisms are then evaluated using chamber observations. Once an explicit mechanism demonstrates agreement with the chamber observations, the chemistry is condensed in stages. The generalizations, deletions, and distortions used to condense the chemistry are evaluated at each step by comparing the predictions of the condensed mechanisms to those of the

FIGURE 1-3: The Development and Evaluation of a Chemical Mechanism


KINETIC AND MECHANISTIC DATA
THEORETICAL CALCULATIONS
Data Evaluation
Assumptions and Deletions
EXPLICIT MECHANISM
Compare Simulations to Chamber Observations
VALIDATED EXPLICIT MECHANISM
Condensation Assumptions
CONDENSED MECHANISM
Compare Simulations to Predictions of Explicit Mechanism
OPERATIONAL CONDENSED MECHANISM

Source: Gery [1987]

explicit mechanism. In this way, a more computationally efficient mechanism is developed with all the important features of the explicit mechanism [Gery, 1987b].

Jeffries [1988d] divides current explicit mechanisms, which represent the state of theoretical knowledge, into four classes of reactions:

(1) a set of inorganic and simple carbonyl reactions for which there is good agreement among researchers as to their rates and products;

(2) a set of organic reactions which have accepted rate constants but uncertain product yields;

(3) a set of organic reactions which are known to occur but for which the rates of reactions, or more likely, the identities of the reaction products are uncertain;

(4) a set of reactions and assumptions used by the modeler to account for the effects of the chamber on the experimental data used to evaluate the mechanism.

Because of the nature of uncertainties in the theoretical knowledge of the rates and products of organic reactions, mechanism testing is performed with a "hierarchy of species." This hierarchy begins with inorganic compounds, at the lowest level, followed by formaldehyde, acetaldehyde, and PAN. Other organic species, such as higher carbonyls, alkanes, alkenes, and aromatics, are added individually and then in simple mixtures. This testing hierarchy decreases the potential for compensating errors which would not be evident if the model were only tested with complex pollutant mixtures [Atkinson et al., 1987].

The condensed mechanisms which result from this development process may be classified by the schemes used to represent the hundreds of hydrocarbon species which are present in urban air. The three mechanisms evaluated in Part 2 represent three different hydrocarbon lumping schemes, summarized in Table 1-4. The CIT mechanism [McRae et al., 1982; Russell et al., 1988a] uses a lumped molecule approach in which all of the species in a certain group are represented by a generalized species whose chemistry is an average of all the species in the group. The CAL mechanism [Carter et al., 1986b; Lurmann et al., 1987] uses a surrogate species approach in which all of the species in a certain group are represented by a specific species in that group. Instead of using the group average, the actual chemistry of the surrogate species represents the chemistry of the entire group. The disadvantage of both of these two approaches is that they do not account for all the carbon in the system. A nine carbon molecule, for instance, may be represented by a seven carbon molecule. To keep track of the amount of carbon, the CB4 mechanism [Gery et al., 1987a] uses a lumped structure approach in which each molecule is broken into its constituent bonds. Each group of bonds goes through a characteristic set of reactions.

TABLE 1-4: Representation of Hydrocarbons in Current Mechanisms

Hydrocarbon Class	Generalized Species CIT	Surrogate Species CAL	Lumped Structure CB4
C4-C5 Alkanes	ALK	ALK4*	PAR
C6+ Alkanes	ALK	ALK7**	PAR
Ethene	ETH	ethene	ETH
Terminal Alkenes	OLE	propene	PAR + OLE
Internal Alkenes	OLE	trans-2-butene	PAR + OLE
Mono-alkylbenzenes	AROM	toluene	TOL
Di-alkylbenzenes	AROM	m-xylene	XYL
Tri-alkylbenzenes	AROM	trimethylbenzene	PAR + XYL
Formaldehyde	HCHO	formaldehyde	HCHO
Acetaldehyde	RCHO	acetaldehyde	ALD2
Higher Aldehydes	RCHO	propionaldehyde	PAR + ALD2

* a mix of n-butane, n-pentane, isobutane, and isopentane

** a mix of n-hexane, n-heptane, n-octane, 2,3-dimethylbutane, 2-methylpentane, 2,3-dimethylpentane, and iso-octane

Species written in upper case letters are theoretical constructs; species written in lower case letters are actual molecules.

Sources: Milford [1988]; Lurmann et al. [1987]; Gery et al. [1987]

Performance of the Current Mechanisms

Ideally, we, the developers and users of photochemical models, would like to believe that the chemical mechanisms are accurate representations of the chemistry which occurs in chamber atmospheres as well as the ambient atmosphere. If this is true, the predictions of the mechanisms should agree with chamber observations for all conditions and all mixtures. Unfortunately, this is not the case. Jeffries et al. [1988a] have compared the predictions of CAL and CB4 to observations from chamber experiments using individual hydrocarbon species and simple mixtures. Their comparison demonstrated that mechanism predictions do not agree with the observations from experiments using individual hydrocarbons as well as they do with observations from experiments using mixtures of hydrocarbons. Furthermore, Jeffries et al. [1988a] have demonstrated that mechanisms may perform well in comparison to ozone observations, but predictions of other products such as HCHO and PAN are not as good. The results of this comparison are summarized in Table 1-5. Note the under prediction of HCHO concentrations for alkenes and the over prediction of HCHO concentrations for aromatics.

Having rejected the ideal condition, we base our belief on the more practical condition that the mechanisms are at

TABLE 1-5: Ability of Current Mechanisms To Model The Fate of Individual Hydrocarbons

Initial Hydrocarbon	Predicted Species	Mechanism Performance CB4	CAL
HCHO	O_3	adequate	adequate
	HCHO	adequate	adequate
ethene	O_3	adequate	adequate
	ethene	adequate	adequate
	HCHO	low	low
propene	O_3	very high	very high
	propene	low	low
	HCHO	low	low
1-butene	O_3	very high	very high
	butene	low	low
	HCHO	high	high
trans-2-butene	O_3	low	low
	butene	very high	very high
	HCHO	low	low
toluene	O_3	adequate	adequate
	toluene	OK/high	OK/high
	HCHO	very high	very high
	PAN	high	high
m-xylene	O_3	high	high
	xylene	adequate	adequate
	HCHO	very high	very high
	PAN	high/low	high/low
o-xylene	O_3	high	high
	xylene	low	low
	HCHO	high/low	high/low
	PAN	low	low

Source: Jeffries [1988]

Note: "Adequate" indicates that model predictions and observed data showed reasonable agreement. "High" and "very high" indicate that the models over predict the observed data. "Low" and "very low" indicate that the models under predict the observed data.

least adequate representations of the conditions and mixtures in which we are interested. Testing this condition is precisely the purpose of this report: Do the current chemical mechanisms adequately predict the concentrations of ozone, formaldehyde, and PAN which result from MFV usage?

Previous Assessments

Several airshed modeling and smog chamber studies have been conducted in the past six years to assess the air quality impacts of MFVs. In 1983, Systems Applications, Inc. (SAI) and the California Institute of Technology (Cal Tech) both conducted modeling assessments of MFV use scenarios in Los Angeles. SAI used the Carbon-Bond Mechanism-III in their assessment, and the CIT mechanism was used by Cal Tech. SAI predicted a 23% reduction in ozone concentrations by 1987 if all motor vehicle hydrocarbon emissions were composed of 89% methanol, 10% formaldehyde, and 1% methyl nitrite. The predicted reduction in ozone concentrations dropped to 13% when the formaldehyde content of the exhaust was raised to 20% [Ballentine, et al. 1985]. Cal Tech assumed a MFV exhaust hydrocarbon composition of 72.7% methanol, 21.2% formaldehyde, and 6.1% alkanes, as well as lower NO_x emission rates compared to conventionally fueled vehicles. Assuming complete conversion of all gasoline-fueled vehicles by the year 2000, they predicted a 14.4 to 20% reduction in peak ozone concentrations. The reduction in ozone was predicted to decrease approximately linearly with the extent of methanol substitution [O'Toole et al., 1983]. Neither assessment predicted significant increases in formaldehyde concentrations [Ballentine et al., 1985].

In 1984, SAI and the University of Santa Clara [Pefley et al., 1984] conducted a series of indoor smog chamber experiments in which one third of a surrogate urban mixture was replaced with a surrogate methanol exhaust. This surrogate exhaust consisted of 90% methanol and 10% isobutene, a surrogate for formaldehyde. The experiments were conducted at three different HC/NO_x ratios--3:1, 9:1, 27:1. For the low and moderate HC/NO_x ratios, the methanol substitution produced a significant decrease in ozone formation over one day. There was not a significant reduction in ozone formation for the highest HC/NO_x ratio. These results were duplicated in a second series of experiments in which one third of the surrogate urban mixture was replaced by exhaust from a vehicle burning fuel of 95% methanol and 5% isopentane.

The data from the chamber experiments were used to develop an extended version of the CBM-III mechanism. Using this extended mechanism, SAI predicted an 18% or more reduction in ozone formation for the Los Angeles basin if all mobile sources in the basin burned M100 fuel by 1987. SAI also predicted a slight increase in peak concentrations of formaldehyde but no significant change in the average ambient concentration.

In 1985, Ballentine et al. conducted a review of the chemical mechanisms and dispersion models available, at that time, to simulate methanol photochemistry. They observed that there is little in the results of the past modeling studies which differentiate the chemical mechanisms used. What little variation there is may be due to the use of different emissions inventories and meteorological conditions and differing assumptions concerning the composition of methanol exhaust, the composition of background hydrocarbons, and the extent of methanol substitution.

In discussing the methanol emissions of concern, Ballentine et al. [1985] suggested that because the only fate of methyl nitrite is photodissociation, its concentration could build up over night as emissions occured. In the morning, relatively large amounts of methyl nitrite and formaldehyde could provide radicals to drive the formation of ozone. Without changing the peak concentration, methanol substitution may increase the integrated exposure to ozone by reaching the peak concentration sooner. Furthermore, Ballentine et al. [1985] suggested that ozone concentrations on the second and third day of a multiple day pollution episode may not experience the same significant reductions due to methanol substitution as the first day.

In 1985, Jeffries, Sexton, and Holleman published the results of a series of side-by-side outdoor chamber experiments conducted at the University of North Carolina (UNC). The experiments were designed to provide a database for evaluating the ability of chemical mechanisms to simulate the impact of large scale substitution of methanol exhaust for automobile exhaust and urban hydrocarbons. These experiments constitute the chamber database for the mechanism evaluation in Part 2 and are described in greater detail in a later section. As predicted by the earlier studies, Jeffries et al. [1985b] observed that the reduction in maximum ozone concentrations resulting from methanol substitution decreased with increasing HC/NO_x ratio and increasing formaldehyde content of the methanol exhaust. For example, there was no difference seen between the ozone levels produced by synthetic auto exhaust with a HC/NO_x ratio of 9:1 and a mixture of 67% synthetic auto exhaust and 33% synthetic methanol exhaust regardless of formaldehyde content. However, for a synthetic urban hydrocarbon mixture with a HC/NO_x ratio of 3:1, 33% replacement with a synthetic methanol exhaust containing no formaldehyde produced a 50% reduction in the peak ozone concentration.

Shortly after the UNC experiments were published, the University of California's Statewide Air Pollution Research Center (SAPRC) published a series of multiple day methanol substitution experiments conducted in both indoor and outdoor chambers [Carter et al., 1986a]. Carter et al. concluded that the formaldehyde content of methanol exhaust and evaporative emissions must be less than 10% to achieve a reduction in ambient ozone concentrations. As in the UNC experiments, methanol substitution resulted in no reduction in ozone concentrations given mixtures with high HC/NO_x ratios. Furthermore, no reduction in ozone concentrations due to methanol substitution was observed after two and three days of irradiation. There was a reduction in PAN concentrations due to the methanol substitution which did not depend on the formaldehyde content of methanol exhaust or on the number of days irradiated. In the case of formaldehyde, Carter et al. [1986a] concluded that methanol substitution will increase ambient concentrations, but that the contribution of methanol exhaust is "relatively moderate" compared to the amount of formaldehyde which results from the reactions of other organic compounds in an urban mixture.

In 1986, SAI conducted an airshed modeling study of methanol substitution in the Philadelphia area [Whitten et al., 1986]. Using the extended version of CBM-III and a projected emissions inventory for the year 2000, they calculated the impact of replacing all gasoline-powered vehicle hydrocarbon emissions with 89% methanol, 10% formaldehyde, and 1% methyl nitrite. The methanol substitution had no significant impact on the predicted maximum ozone concentrations, partly due to the low contribution of mobile sources to the total hydrocarbon emissions in the Philadelphia area. As the HC/NO_x ratio was decreased, however, predicted peak ozone concentrations decreased. The production of PAN and other nitrogenous organic species was predicted to decrease due to the methanol substitution. Formaldehyde concentrations were predicted to increase by less than 20% depending on the contribution of mobile sources to the total VOC emissions. Whitten et al. [1986] noted that as the reactivity of the VOC emissions or the total amount of VOC emissions decreases the ozone contribution of formaldehyde becomes more important .

Currently, researchers at Carnegie-Mellon University (CMU) have completed the first two phases of a three-tiered modeling study of methanol fuel usage in the Los Angeles basin. In the first phase of the study, Russell and Harris [1988b] compared the predictions of the CIT mechanism to the observations made in the SAPRC experiments described above. Good agreement was seen between the predicted and observed peak ozone concentrations over two days of the multiple day experiments. The ozone formation sensitivity of the CIT mechanism was compared to that of the CAL mechanism and was found to have similar sensitivites to changes in methanol and formaldehyde concentrations. Russell and Harris [1988b] concluded, therefore, that the CIT mechanism is appropriate for modeling the impact of MFVs. In the second phase of the study, Russell and Harris [1988b] used the CIT mechanism in a Lagrangian model to simulate 70 emission scenarios along three multiple day trajectories. MFV usage resulted in reduced ozone concentrations in all cases; as in all the previous studies, the magnitude of the reduction was found to be dependent on the HC/NO_x ratio. In contrast to previous studies, however, the trajectory calculations showed very little sensitivity to varying the formaldehyde content of the MFV exhaust between 1% and 10% by mass. Russell and Harris [1988b] did not make any predictions regarding ambient concentrations of formaldehyde or PAN. In the third phase of the modeling study, which is currently being completed, an Eulerian airshed model is being used to evaluate the conclusions of the trajectory modeling.

Current Uncertainties

There is a great deal of consistency among the results of the previous impact assessments. It is clear that the ozone reduction achieved by using MFVs is variable depending on the ambient hydrocarbon mixture, the contribution of mobile sources, and the amount of formaldehyde emitted. While the CMU study should provide some answers to the questions concerning the effects of MFVs on multiple day ozone episodes, the impact of MFVs on ambient formaldehyde and PAN concentrations remains uncertain.

Part 2

A Restatement of the Purpose

Part 1 of this report has dealt with four preliminary issues: the emissions that can be expected from MFVs, the air quality impacts of concern, the need for mechanism testing, and the findings of past MFV assessments. With this information, the basic purpose of this report becomes more defined: to evaluate the ability of current photochemical mechanisms to predict ozone and PAN maximum concentrations and HCHO concentration profiles in chamber experiments in which a fraction of typical urban hydrocarbons are replaced by mixtures of methanol and formaldehyde.

The Chamber Experiments

The chamber experiments which will serve as the basis of the mechanism evaluation come from the work of Jeffries, Sexton, and Holleman [1985b] discussed in Part 1. The experiments are part of over 280 experiments which have been conducted in the University of North Carolina's Outdoor Smog Chamber in rural North Carolina. The 300,000 liter chamber consists of a wood and aluminum A-frame skeleton that supports sheets of 5-mil Fluorinated Ethylene Propylene (FEP) Teflon film. A vertical piece of film divides the chamber into two halves allowing side by side comparisons of different air mixtures. The floor of the chamber is backed with aluminum foil to reflect light and heat back up through the chamber. The chamber is equipped with multiple air handling systems which allow for intake, exhaust, mixing, and dehumidifying of the chamber air and sampling and injection of pollutant materials. Analytical instrumention and calibration systems are housed in an adjacent laboratory and are time-shared by the two sides of the chamber.

The selected experiments were designed to simulate the effect of changing the composition of pollutant emissions by injecting a control mixture into one side of the chamber, and a different mixture into the other side. Because both sides of the chamber are exposed to the same ambient sunlight, temperature, and humidity conditions and are sampled by the same set of instruments, the differences in the observations between the two sides can be attributed to the difference in the chemical mixtures. The two sides of the chamber have been designated as red and blue for identification purposes. For purposes of discussion, I will refer to the two sides as the control side and the reduction/substitution side depending on the chemical mixture present.

As explained in Part 1, two control mixtures were used in this set of experiments: SynAuto, a synthetic auto exhaust derived from previous comparison work in the UNC chamber, and SynUrban, a synthetic urban air mixture derived from emissions inventories and atmospheric measurements. The species compositions of these two mixtures are given in Table 2-1.

An initial NO_x concentration of approximately 0.35 ppm was used in all of the experiments. Two HC/NO_x ratios, 9/1 and 3/1, were achieved by varying the initial concentration of each of the hydrocarbon mixtures.

On the one side of the chamber, the control mixtures were changed by either reducing the initial hydrocarbon concentration by 33% or by replacing 33% of the mixture with a synthetic methanol exhaust. The composition of the synthetic methanol exhaust was varied between three mixtures of methanol and formaldehyde: 80% MeOH/20% HCHO, 90%MeOH/10% HCHO, and 100% MeOH. In four of the experiments, 1% of the methanol was replaced with methyl nitrite.

TABLE 2-1: Composition of Hydrocarbon Mixtures

Compound	SynAuto	SynUrban
n-butane	0.0391	0.1000
n-pentane		0.1367
isopentane	0.0519	0.0801
2-methylpentane		0.0538
2,4-dimethylpentane		0.0467
2,2,4-trimethylpentane	0.1121	0.1340
ethylene	0.2391	0.0630
propylene	0.0416	0.0238
1-butene	0.0196	0.0137
trans-2-butene	0.0196	
cis-2-butene		0.0169
2-methyl-1-butene		0.0187
2-methyl-2-butene		0.0171
benzene	0.0538	0.0331
toluene	0.2115	0.1304
m-xylene	0.1026	0.0633
o-xylene	0.0481	0.0296
1,2,4-trimethylbenzene	0.0564	0.0347
formaldehyde	0.0200	0.0200

Source: Jeffries et al. [1985b]

Several additional experiments were conducted with a mixture of intermediate reactivity designated SynAutoUrb and consisting of 90% SynAuto and 10% n-butane. One experiment was conducted using only the high molecular weight portion of the SynAuto and SynUrban mixture. This mixture consisted of 80% aromatics and 20% trimethylpentane and was designated HMWMIX.

A summary of the initial conditions for the chamber experiments selected for the mechanism evaluation is given in Table 2-2.

The standard procedure for the experiments began by flushing the chamber and filling it with rural ambient air overnight. Before dawn, the chamber was sealed, the enclosed air was circulated through dehumidifiers, and the monitoring of pollutant concentrations was begun. The initial concentrations of pollutants were injected into the chamber, and the chamber was exposed to natural sunlight and ambient temperature. The chamber air was diluted over the course of the day with ambient air to simulate an atmospheric mixing height rise. Monitoring of the pollutant concentrations continued until about 6:00 PM local daylight time.

The two sides of the chamber were monitored by the following instruments: six packed column and two capillary gas chromatographs for measuring hydrocarbons, organic nitrates, and inert tracer species; a liquid chromatograph for DNPH-aldehyde analysis; an automated wet chemical

TABLE 2-2: Conditions of the Selected UNC Chamber Experiments

HC/NOx Ratio	Control Mixture	Reduction or Substitution	Date
9:1	SynAuto	1/3 HC reduction	Au0684
		1/3 MEOH w/20% HCHO	Au0884
	SynUrban	1/3 HC reduction	Jn2685
		1/3 MEOH w/ 0% HCHO	St0184
		1/3 MEOH w/20% HCHO	Au2284
3:1	SynAuto	1/3 HC reduction	Au0584
		1/3 MEOH w/ 0% HCHO	Au0784
		1/3 MEOH w/10% HCHO	Au0484
		1/3 MEOH w/20% HCHO	Au0984
	SynUrban	1/3 HC reduction	St0284
		1/3 MEOH w/10% HCHO	Au2584
		1/3 MEOH w/10% HCHO	Jn2885
		1/3 MEOH w/20% HCHO	St0384
9:1	SynAutoUrban	1/3 HC reduction	St0884
		1/3 MEOH w/10% HCHO	St1784
		HCHO addition	St2184
	HMWMIX	1/3 HC reduction	St1984

formaldehyde instrument; two chemiluminescent monitors for measuring ozone and NO$_x$; and one UV ozone photometer. Total solar radiation (TSR) and ultraviolet radiation (UV) were measured by sensors mounted on a 7 meter tower next to the laboratory, and chamber air temperature was measured by thermistors inside the chamber sampling manifolds. All of the analytical instruments were calibrated at two concentrations. A baseline concentration was established by sampling from a zero air generator or from a species specific filter. A second calibration point was established by sampling NBS-traceable sources or other commercially available sources. The calibration data for the entire experimental season is compiled and analyzed before it is used to adjust the observed concentrations. Further description of the chamber, analytical systems, and data processing procedures may be found in Jeffries, Sexton, and Holleman [1985b].

Recent work has led to the development of a series of models which describe the light characteristics of the chamber [Jeffries et al., 1988c]. The models compute both the tower irradiances and the in-chamber actinic flux using the time of day, air pressure, total column ozone, total column water vapor, relative humidity, aerosol type, aerosol optical density at 500 nm, and the spectral albedo of the ground. The series of models accounts for the position of the sun, the atmospheric transmission of total solar radiation and ultraviolet radiation, the transmission characteristics of FEP Teflon film, the geometry of the chamber, the effect of the reflective floor, and the effect of clouds. These models were used to predict the tower irradiances for each of the experiments in the UNC database. After the tower irradiances were successfully predicted, the in-chamber actinic fluxes were predicted for every 16 minutes after sunrise. The computed actinic fluxes were then used with species absorption cross sections and reaction quantum yields to compute in-chamber photolysis rates for up to 20 reactions for each experiment. The photolysis rate files for each of the selected experiments are given in Appendix C of this report.

The Mechanisms

The mechanisms that were selected for this evaluation are the three mechanisms whose hydrocarbon lumping schemes were briefly described in Part 1: the Carter, Atkinson, Lurmann mechanism (CAL); the Carbon Bond Mechanism-IV (CB4); and the California Institute of Technology mechanism (CIT). CB4 and CAL are the products of a long-term research program sponsored by the U.S. Environmental Protection Agency for the development of accurate models of urban atmospheric chemistry. Representing the state of the art, these two mechanisms are the focus of this evaluation. CIT was included in this evaluation because of its use in the most recent modeling assessment of methanol fuel impacts [Russell and Harris, 1988b].

Carter, Atkinson, Lurmann Mechanism

CAL was developed by the University of California's Statewide Air Pollution Research Center (SAPRC) and Environmental Research and Technology, Inc. (ERT) [Carter et al., 1986b; Lurmann et al., 1987]. It was developed with smog chamber data from SAPRC and the UNC chamber, including experiments conducted with the SynAuto and SynUrban mixtures. The mechanism has 50 species and 131 reactions, and it utilizes a surrogate species approach to represent hydrocarbons. The mechanism listing used in the chamber simulations is given in Table 2-3. This version is the same as that listed in Jeffries et al. [1988a] and differs from the listing given in Table 2-2 of Lurmann et al. [1987] in several ways: (1) The photolytic reaction rates are those calculated by Jeffries et al. [1988c]. The only significant difference in these rates and those used by Carter et al. [1986b] lies in the choice of absorption cross section data for formaldehyde. Jeffries et al. [1988c] chose to use the Bass cross sections for formaldehyde, as do the developers of CB4. Carter et al. [1986b] prefer to use an average of Bass and Moortgat values. (2) The rate of reaction 2 was incorrectly listed and has been corrected. (3) The rate of reaction 11 has been changed from 1.9 x 10-6 to 1.4 x 10-5 ppm-1 min-1. This reaction is a surface phenomenon and the rate has been increased to account for the larger surface area present in the chamber. (4) The rates of reactions 17 and 18 have been multiplied by 10-5 to ease the numerical solution of the resulting equations. This change has no impact on the calculated concentrations. (5) Reaction 21, which represents the dark formation of HONO from NO2 on the chamber walls, has been omitted so that assumptions about wall processes can be treated seperately. (6) Reaction 50, which summarizes the HCHO-FROX-FACID cycle, overestimates the back reaction and, therefore, has been replaced by three more explicit reactions whose rates agree with the rates used in CB4. (7) Jeffries et al. [1988a] chose to use a value of 15000 ppm-1 min-1 for the rate of reaction 52, as opposed to 13300 ppm-1 min-1.

TABLE 2-3: CAL Mechanism

```
Carter, Atkinson, Lurman, Chamber Version 3.2
(*****************************************************************
Compiled from Lurmann, et al. (1987) "A Surrogate Species Chemical
Reaction Mechanism For Urban-Scale Air Quality Simulation Models:
Volume II--Guidelines for Using the Mechanism."

Modified according to Jeffries, et al. (1988) "Validation
Testing of New Mechanisms with Outdoor Chamber Data:  Volume 1--
Comparison of CB4 and CAL Mechanisms."
*****************************************************************)

( INORGANIC CHEMISTRY )
(  1)          NO2  = NO    + O               # 1.00/L1;
(  2)          O    = O3                      # 8.3E+4@ 1282;
(  3) O     + NO2  = NO                       # 1.37E+04;
(  4) O     + NO2  = NO3                      # 164.06@ 894;
(  5) NO    + O3   = NO2                      # 2.57877E+03@ -1370.;
(  6) NO2   + O3   = NO3                      # 1.67980E+02@ -2450.;
(  7) NO    + NO3  = 2.*NO2                   # 1.18720E+04@ 252.;
(  8) NO    + NO   = 2.*NO2                   # 2.45205E-05@ 529.;
(  9) NO2   + NO3  = N2O5                     # 6.902E+2@ 270;
( 10)          N2O5 = NO2   + NO3             # 1.11E+16 @ -10790.;
( 11) N2O5(+ H2O)  = 2.*HNO3                  # 1.4E-5/W;
                                          (changed from E-6 for chamber)
( 12) NO2   + NO3  = NO    + NO2              # 3.59634E+01@ -1229.;
( 13)          NO3  = NO                      # 0.043/L6;
( 14)          NO3  = NO2   + O               # 0.385/L6;
( 15)          O3   = O                       # 0.001/L6;
( 16)          O3   = O1D                     # 0.001/L4;
( 17) O1D (+ H2O)  = 2.*OH                    # 3.260(1E+5)/W;
( 18)          O1D  = O                       # 4.32E+5(1E+5);
                                   (multiplied by E-5 to lower stiffness)
( 19) NO    + OH   = HONO                     # 1.06528E+03@ 670.;
( 20)          HONO = NO    + OH              # 0.171/L1;

(This reaction has been omitted and the original Carter chamber
radical treatment has been added.
( 21)NO2 (+ H2O)   = HONO + -1.*NO2   + HNO3   #1.17E-04;)

( 22) NO2   + OH    = HNO3                    # 2.18674E+03@ 617.;
( 23) HNO3 + OH     = NO3                     # 1.41316E+01@ 778.;
( 24) CO    + OH    = HO2                     # 3.22E+02;
( 25) O3    + OH    = HO2                     # 2.31039E+03@ -942.;
( 26) NO    + HO2   = NO2   + OH              # 5.48181E+03@ 240.;
( 27) NO2   + HO2   = HNO4                    # 2.49368E+02@ 632.;
( 28)         HNO4  = NO2   + HO2             # 4.2E+15@ -10240.;
( 29) HNO4 + OH     = NO2                     # 5.91E+03;
( 30) O3    + HO2   = OH                      # 2.03930E+01@ -579.;
( 31) HO2   + HO2   = H2O2                    # 3.41349E+02@ 771.;
( 32) HO2   + HO2 (+ H2O) = H2O2              # 2.52539E-01@ 2971.;
( 33) NO3   + HO2   = HNO3                    # 3.41349E+02@ 771.;
( 34) NO3   + HO2 (+ H2O) = HNO3              # 2.52539E-01@ 2971.;
( 35)         H2O2  = 2.*OH                   # 0.293E-3/L2;
( 36) H2O2 + OH     = HO2                     # 4.56958E+03@ -187.;
( GENERALIZED RO2 CHEMISTRY -- LOSS STEPS )
( 37) RO2  + NO   = NO                      # 8.25645E+03@ 180.;
( 38) RCO3 + NO   = NO                      # 8.25645E+03@ 180.;
( 39) RCO3 + NO2  = NO2                     # 4.15450E+03@ 180.;
( 40) RO2  + HO2  = HO2                     # 4.43E+03;
( 41) RCO3 + HO2  = HO2                     # 4.43E+03;
( 42)        ROOH = HO2  + OH               # 0.294E-3/L2;
( 43) RO2  + RO2  =                         # 1.48E+00;
( 44) RO2  + RCO3 =                         # 4.43E+03;
( 45) RCO3 + RCO3 =                         # 3.69E+03;

( CARBONYL CHEMISTRY )
      ( Formaldehyde )
( 46)        HCHO = 2.*HO2  + CO            # 0.001/L2;
( 47)        HCHO = CO                      # 0.001/L3;
( 48) HCHO + OH   = HO2  + CO               # 1.50E+04;
                                    (changed from 1.33E+04)
( 49) HCHO + NO3  = HNO3 + HO2  + CO        # 8.46494E+02@ -2060.;

(50a) HCHO + HO2  = FROX                    # 1.48E+01;
(50b)        FROX = HCHO + HO2              # 90.0;
(50c) FROX + NO   = NO2  + HO2 (+FACID)     # 8.25645E+03@ 180.;
(The original reaction was ...
( 50) HCHO + HO2  = RO2R + RO2              # 1.48E+01;
 ... which omitted the back reaction and overestimated the
pathway.)

    ( Acetaldehyde )
( 51) ALD2 + OH   = MCO3 + RCO3             # 1.02565E+04@ 250.;
( 52)        ALD2 = CO   + HCHO + HO2  + RO2R + RO2
                                            # 0.001/L5;
( 53) ALD2 + NO3  = HNO3 + MCO3 + RCO3      # 4.29359E+02@ -1427.;
( 54) MCO3 + NO   = NO2  + HCHO + RO2R + RO2
                                            # 8.25645E+03@ 180.;
( 55) MCO3 + NO2  = PAN                     # 4.15450E+03@ 180.;
( 56) MCO3 + HO2  = ROOH + HCHO             # 4.43E+03;
( 57) MCO3 + RO2  = .5*HO2  + HCHO + RO2    # 4.43E+03;
( 58) MCO3 + RCO3 = HO2  + HCHO + RCO3      # 3.69E+03;
( 59)        PAN  = MCO3 + NO2  + RCO3      # 1.2014926E+18@ -13550.;

    ( Higher Aldehyde )
( 60) RCHO + OH   = RCO3 + PCO3             # 1.26468E+04@ 250.;
( 61)        RCHO = ALD2 + HO2  + CO   +    RO2R + RO2
                                            # 0.0023/L5;
( 62) RCHO + NO3  = HNO3 + PCO3 + RCO3      # 4.29359E+02@ -1427.;
( 63) PCO3 + NO   = NO2  + ALD2 + RO2R +    RO2
                                            # 6.25645E+03@ 180.;
( 64) PCO3 + NO2  = PPN                     # 4.15450E+03@ 180.;
( 65) PCO3 + HO2  = ROOH + ALD2             # 4.43E+03;
( 66) PCO3 + RO2  = .5*HO2  + ALD2 + RO2    # 4.43E+03;
( 67) PCO3 + RCO3 = HO2  + ALD2 + RCO3      # 3.69E+03;
( 68)        PPN  = PCO3 + NO2  + RCO3      # 8.87304E+17@ -13550.;

    ( Acetone )
( 69)        ACET = MCO3 + HCHO + RCO3 +    RO2R + RO2
                                            # 0.2E-3/L1;
( 70) ACET + OH   = MGLY + RO2R + RO2       # 1.44146E+04@ -1125.;
```

```
    ( Ketones )
( 71)         MEK   = MCO3 + ALD2 + RCO3 + RO2R + RO2
                                             # 3.5E-3/L5;
( 72) MEK   + OH    = 1.5*R2O2 + 1.5*RO2  + .5*MCO3 +
                      .5*ALD2 + .5*HCHO + .5*PCO3 + RCO3
                                             # 1.74925E+04@ -745.;

    ( Glyoxal )
( 73)         GLYX = .13*HCHO + 1.87*CO    # 0.011/L1;
( 74) GLYX + OH    = .63*HO2  + 1.26*CO    + .37*GCO3 + .37*RCO3
                                           # 1.70E+04;
( 75) GLYX + NO3   = HNO3 + .63*HO2  + 1.26*CO   +
                     .37*GCO3 + .37*RCO3   # 8.46494E+02@ -2060.;
( 76) GCO3 + NO2   = GPAN                  # 4.15450E+03@ 180.;
( 77) GCO3 + NO    = NO2  + HO2  + CO      # 6.25645E+03@ 180.;
( 78)         GPAN = GCO3 + NO2  + RCO3    # 8.87304E+17@ -13550.;
( 79) GCO3 + HO2   = ROOH + CO             # 4.43E+03;
( 80) GCO3 + RO2   = .5*HO2  + CO   + RO2  # 4.43E+03;
( 81) GCO3 + RCO3  = HO2  + CO   + RCO3    # 3.69E+03;

    ( Methyl glyoxal )
( 82)         MGLY = MCO3 + HO2  + CO   + RCO3
                                           # 0.021/L1;
( 83) MGLY + OH    = MCO3 + CO   + RCO3    # 2.51E+04;
( 84) MGLY + NO3   = HNO3 + MCO3 + CO   + RCO3
                                           # 4.29359E+02@ -1427.;

( PARAFFIN CHEMISTRY )
( 85) ALK4 + OH    = .19*HCHO + .305*ALD2 + .163*RCHO +
                     .34*ACET + .445*MEK  + .0757*RO2N +
                     .924*RO2R + .589*R2O2 + 1.51*RO2
                                           # 1.54257E+04@ -354.;
( 86) ALK7 + OH    = .0218*HCHO + .0313*ALD2 + .247*RCHO +
                     .351*ACET + .874*MEK  + .197*RO2N +
                     .803*RO2R + .825*R2O2 + 1.63*RO2
                                           # 2.37934E+04@ -289.;

( 87) ALKN + OH    = NO2  + .15*MEK  + 1.05*RCHO +
                     .48*ALD2 + .16*HCHO + 1.39*R2O2 +
                    1.39*RO2               # 3.18782E+04@ -711.;

( GENERALIZED RO2 CHEMISTRY -- OXIDATION STEPS )
( 88) RO2N + NO    = ALKN                  # 6.25645E+03@ 180.;
( 89) RO2N + HO2   = ROOH + MEK            # 4.43E+03;
( 90) RO2N + RO2   = RO2  + .5*HO2  + MEK  # 1.48E+00;
( 91) RO2N + RCO3  = RCO3 + .5*HO2  + MEK  # 4.43E+03;

( 92) R2O2 + NO    = NO2                   # 6.25645E+03@ 180.;
( 93) R2O2 + HO2   = ROOH                  # 4.43E+03;
( 94) R2O2 + RO2   = RO2                   # 1.48E+00;
( 95) R2O2 + RCO3  = RCO3                  # 4.43E+03;

( 96) RO2R + NO    = NO2  + HO2            # 6.25645E+03@ 180.;
( 97) RO2R + HO2   = ROOH                  # 4.43E+03;
( 98) RO2R + RO2   = .5*HO2  + RO2         # 1.48E+00;
( 99) RO2R + RCO3  = .5*HO2  + RCO3        # 4.43E+03;
( OLEFIN CHEMISTRY )
   ( Ethylene )
(100) ETHE + OH    = RO2R + RO2   + 1.56*HCHO + .22*ALD2
                                          # 3.20175E+03@ 411.;
(101) ETHE + O3    = HCHO + .12*HO2   + .42*CO
                                          # 1.67124E+01@ -2634.;
(102) ETHE + O     = HCHO + HO2   + CO + RO2R + RO2
                                          # 1.51343E+04@ -792.;
(103) ETHE + NO3   = NO2   + 2.*HCHO + R2O2 + RO2
                                          # 2.76183E+03@ -2925.;

   ( Propylene )
(104) PRPE + OH    = RO2R + HCHO + ALD2 + RO2
                                          # 7.24995E+03@ 504.;
(105) PRPE + O3    = .65*HCHO + .5*ALD2   + .285*CO   +
                     .06*OH    + .165*HO2  + .135*RO2R +
                     .135*RO2             # 1.86216E+01@ -2105.;
(106) PRPE + O     = .6*ACET + .4*HCHO + .2*ALD2 +
                     .2*HO2   + .6*RO2R + .4*CO   +
                     .6*RO2               # 1.73147E+04@ -324.;
(107) PRPE + NO3   = NO2   + HCHO + ALD2 + R2O2 + RO2
                                          # 7.08627E+03@ -1935.;

   ( Trans-2-butene )
(108) TBUT + OH    = RO2R + 2.*ALD2 + RO2     # 1.51110E+04@ 549.;
(109) TBUT + O3    = ALD2 + .15*CO    + .27*RO2R +
                     .12*OH    + .21*HO2   + .27*RO2 + .30*HCHO
                                              # 1.30999E+01@ -1137.;
(110) TBUT + O     = MEK   + .4*HO2           # 3.33690E+04@ 10.;
(111) TBUT + NO3   = NO2   + 2.*ALD2 + R2O2 + RO2
                                              # 1.44684E+04@ -975.;

( AROMATICS CHEMISTRY )
(112) TOLU + OH    = .16*CRES + .16*HO2   + .84*RO2R +
                     .4*DIAL + .84*RO2   + .144*MGLY +
                    .114*GLYX                 # 3.12492E+03@ 320.;

(113) XYLE + OH    = .17*CRES + .17*HO2   + .83*RO2R +
                     .83*RO2   + .65*DIAL + .316*MGLY +
                    .095*GLYX                 # 2.45913E+04@ 116.;

(114) TMBZ + OH    = .17*CRES + .17*HO2   + .83*RO2R +
                     .83*RO2   + .49*DIAL + .86*MGLY
                                              #9.16E+04;

(115) DIAL + OH    = PCO3 + RCO3              # 4.43E+04;
(116)          DIAL = HO2   + CO    + MCO3 + RCO3
                                              # 0.060/L1;

(117) CRES + OH    = .2*MGLY + .15*RO2P + .85*RO2R + RO2
                                              # 5.91E+04;
(118) CRES + NO3   = HNO3 + BZO               #3.25E+04;

(119) RO2P + NO    = NPHE                     # 6.25645E+03@ 180.;
(120) RO2P + HO2   = ROOH                     # 4.43E+03;
(121) RO2P + RO2   = .5*HO2   + RO2           # 1.48E+00;
```

```
(122) RO2P + RCO3 = .5*HO2  + RCO3                 # 4.43E+03;

(123) BZO  + NO2  = NPHE                           # 2.22E+04;
(124) BZO  + HO2  = PHEN                           # 4.43E+03;
(125)        BZO  = PHEN                           # 6.00E-02;
(126) PHEN + OH   = .2*GLYX + .15*RO2P + .85*RO2R + RO2
                                                   # 4.14E+04;
(127) PHEN + NO3  = HNO3 + BZO                     # 5.62E+03;
(128) NPHE + NO3  = HNO3 + BZN2                    # 5.62E+03;
(129) BZN2 + NO2  =                                # 2.22E+04;
(130) BZN2 + HO2  = NPHE                           # 4.43E+03;
(131)        BZN2 = NPHE                           # 6.00E-02;
```

Carbon Bond Mechanism-IV

CB4 was developed by Systems Applications, Inc., (SAI) and is currently the default mechanism for the EPA's EKMA model [Gery et al., 1987a]. It was developed using experimental data from four smog chambers including the SAPRC and UNC chambers. While the selected set of methanol experiments were not used in the development process, experiments using the SynAuto and SynUrban mixtures were. The mechanism has 81 reactions and 33 species, and it utilizes the lumped structure approach to represent hydrocarbons. The mechanism listing used in the chamber simulations is the same as that listed in Jeffries et al. [1988a] and is given in Table 2-4. This listing differs from the listing given in Table 1-3 of Gery et al. [1987a] in two ways: (1) The photolytic reaction rates are those calculated by Jeffries et al. [1988c]. (2) As for CAL reaction (11), the rate of reaction (18) has been changed from 1.9×10^{-6} to 1.4×10^{-5} ppm^{-1} min^{-1}.

TABLE 2-4: CB4 Mechanism

```
Carbon Bond Four.Two, Chamber Version Sub3.2
(*************************************************************
Compiled from Gery, et al. (1988) "Development and Testing of the
CBM-IV for Urban and Regional Modeling." Atmospheric Sciences
Research Laboratory, U.S. Environmental Protection Agency, EPA
600/3-88-012.

Modified according to Jeffries, et al. (1988) "Validation Testing
of New Mechanisms with Outdoor Chamber Data:  Volume 1--Comparison
of CB4 and CAL Mechanisms."
**************************************************************)

   ( INORGANIC CHEMISTRY )
(  1)               NO2     = NO    + O          # 1.0   /L1        ;
(  2) O    (+ O2    + M   ) = O3    (+ M   )     # 83830.    @ 1175.;
(  3) O3    + NO            = NO2   (+ O2  )     # 2.643E+03 @-1370.;

(  4) O     + NO2           = NO    (+ O2  )     # 1.375E+04        ;
(  5) O     + NO2 (+ M    ) = NO3   (+ M   )     # 230.3     @ 687. ;
(  6) O     + NO  (+ M    ) = NO2   (+ M   )     # 323.3     @ 602. ;

(  7) O3    + NO2           = NO3   (+ O2  )     # 176.00    @-2450. ;
(  8) O3                    = O     (+ O2  )     # 0.001/L6          ;
(  9) O3                    = O1D   (+ O2  )     # 0.001/L4          ;
( 10) O1D (+ M            ) = O     (+ O2  )     # 1.147E+5 @ 390.   ;
( 11) O1D (+ H2O          ) = 2.0*OH             # 3.26/W            ;
( 12) O3    + OH            = HO2   (+ O2  )     # 2344.     @-940.  ;
( 13) O3    + HO2           = OH    (+ 2O2 )     # 21.0      @-580.  ;

   ( NO3 CHEMISTRY )
( 14)         NO3          = 0.89*NO2 + 0.89*O + 0.11*NO
                                                 # 0.428/L6          ;
( 15) NO3   + NO           = 2.0*NO2             # 19090     @ 250.  ;
( 16) NO3   + NO2          = NO     + NO2        # 36.6      @-1230. ;
( 17) NO3   + NO2 (+ M    ) = N2O5 (+ M      )   # 784.9     @ 256.  ;
( 18) N2O5 (+ H2O         ) = 2.0*HNO3           # 1.4E-5/W          ;
                               (changed from 1.9E-6 for chamber)
( 19) N2O5 (+ M           ) = NO3 + NO2 (+M   )  # 2.11E+16 @-10897.;
( 20) NO    + NO  (+ O2   ) = 2.0*NO2            # 2.60E-5  @ 530.  ;

   ( HONO CHEMISTRY )
( 21) NO    + NO2 (+ O2   ) = 2.0*HONO           # 1.6E-11/W         ;
( 22) OH    + NO  (+ M    ) = HONO (+ M       )  # 655.44    @ 806.  ;
( 23)         HONO          = OH    + NO         # 0.171/L1          ;
( 24) OH    + HONO          = NO2  (+ H2O     )  # 9770.             ;
( 25) HONO + HONO           = NO    + NO2 (+H2O) # 1.5E-5            ;

( 26) OH    + NO2 (+ M    ) = HNO3               # 1537.     @ 713.  ;
( 27) OH    + HNO3          = NO3                # 7.6       @ 1000. ;
( 28) HO2   + NO            = OH    + NO2        # 5482.     @ 240.  ;
( 29) HO2   + NO2 (+ M    ) = PNA  (+ M       )  # 164.0     @ 749.  ;
( 30) PNA   (+ M          ) = HO2 + NO2 (+M   )  # 2.876E+15 @-10121.;
( 31) OH   + PNA           = NO2 (+H2O  + O2 ) # 1909.     @ 380.  ;

( 32) HO2  + HO2           = H2O2 (+ O2)       # 87.39     @ 1150.;
( 33) HO2  + HO2 (+ H2O )  = H2O2 (+ O2 + H2O) # 7.69E-10 @ 5800./W;
( 34)            H2O2      = 2*OH              # 0.293E-3/L2       ;
( 35) OH   + H2O2          = HO2  (+ H2O     ) # 4720.     @-187   ;

( 36) OH   + CO  (+ M   )  = HO2  (+ CO2     ) # 322.0             ;

 ( FORMALDHYDE CHEMISTRY )
( 37) HCHO + OH   = HO2   + CO                 # 15000             ;
( 38)          HCHO = 2*HO2 + CO               # 0.001/L2          ;
( 39)          HCHO = CO                       # 0.001/L3          ;
( 40) HCHO + O    = OH    + HO2 + CO           # 4302.     @-1550  ;
( 41) HCHO + NO3  = HNO3 + HO2 + CO            # 0.93              ;

 ( HIGHER ALDEHYDE CHEMISTRY )
( 42) RCHO + O    = C2O3 + OH                  # 17394.7   @-986   ;
( 43) RCHO + OH   = C2O3                       # 10370.    @ 250   ;
( 44) RCHO + NO3  = C2O3 + HNO3                # 3.7               ;
( 45)        RCHO = XO2  + 2*HO2 + CO + HCHO   # 0.001/L5          ;

 ( PAN CHEMISTRY )
( 46) C2O3 + NO   = NO2  + XO2 + HCHO + HO2    # 7915.0    @ 250   ;
( 47) C2O3 + NO2  = PAN                        # 0.000118  @ 5500  ;
( 48)        PAN  = C2O3 + NO2                 # 5.616E18  @-14000;

( 49) C2O3+ C2O3  = 2*XO2 + 2*HCHO + 2*HO2     # 3700              ;
( 50) C2O3+ HO2   = 0.79*HCHO + 0.79*XO2 + 0.79*HO2 + 0.79*OH
                                               # 9600              ;
( 51) OH  (+ CH4)        = XO2 + HCHO + HO2    # 6521      @-1710  ;

 ( PARAFFIN CHEMISTRY )
( 52) OH   + PAR  = 0.87*XO2 + 0.13*XO2N + 0.11*HO2 + 0.11*RCHO
                    + 0.76*ROR + -0.11*PAR     # 1203.0            ;
( 53)        ROR  = 1.1*RCHO + 0.96*XO2 + 0.94*HO2 + -2.1*PAR
                    + 0.04*XO2N + 0.02*ROR     # 6.25E+16  @-8000  ;
( 54)        ROR  = HO2 (+ KET)                # 95450.            ;
( 55) ROR + NO2   = (NTR)                      # 22000.            ;

 ( OLEFIN CHEMISTRY )
( 56)  O   + OLE  = 0.63*RCHO + 0.38*HO2 + 0.28*XO2 + 0.30*CO
                  + 0.20*HCHO + 0.02*XO2N + 0.22*PAR + 0.20*OH
                                               # 17560.0   @-324   ;
( 57) OH   + OLE  = HCHO + RCHO + XO2 + HO2 + -1*PAR
                                               # 7740.0 @ 504      ;
( 58) O3   + OLE  = 0.5*RCHO + 0.74*HCHO + 0.33*CO + 0.44*HO2
                  + 0.22*XO2 + 0.10*OH + -1.0*PAR
                                               # 21.04     @-2105  ;
( 59) NO3 + OLE   = 0.91*XO2 + 0.09*XO2N + HCHO + RCHO + -1*PAR
                  + NO2                        # 11.35             ;
```

```
  ( ETHYLENE CHEMISTRY )
( 60) O    + ETH   = HCHO + 0.70*XO2 + CO + 1.70*HO2+ 0.30*OH
                                                # 15400     @-792  ;
( 61) OH   + ETH   = XO2 + 1.56*HCHO + HO2 + 0.22*RCHO
                                                # 3000      @ 411  ;
( 62) O3   + ETH   = HCHO + 0.42*CO + 0.12*HO2 # 18.56     @-2633 ;

  ( TOLUENE CHEMISTRY )
( 63) OH    + TOL  = 0.08*XO2 + 0.36*CRES + 0.44*HO2 + 0.56*TO2
                                                # 3106.     @322.  ;
( 64) TO2   + NO   = 0.90*NO2 + 0.90*HO2 + 0.90*OPEN
                                                # 12000.           ;
( 65) TO2          = CRES + HO2                 # 250              ;
( 66) OH    + CRES = 0.4*CRO + 0.60*XO2 + 0.60*HO2 + 0.30*OPEN
                                                # 61000            ;
( 67) NO3   + CRES = CRO + HNO3                 # 32500            ;
( 68) CRO   + NO2=                              # 20000            ;
( 69) OPEN         = C2O3 + HO2 + CO            # 0.021/L1         ;
( 70) OPEN + OH = XO2 + 2.0*CO + 2.0*HO2 + C2O3 + HCHO
                                                # 44000.           ;
( 71) OPEN + O3 = 0.03*RCHO + 0.62*C2O3 + 0.70*HCHO + 0.03*XO2
                + 0.69*CO + 0.08*OH + 0.76*HO2 + 0.2*MGLY
                                                # 0.0803    @-500. ;

  ( XYLENE CHEMISTRY )
( 72) OH    + XYL = 0.70*HO2 + 0.50*XO2 + 0.20*CRES + 0.80*MGLY
                  + 1.10*PAR + 0.30*TO2         # 24530.    @ 116. ;

  ( DICARBONYL CHEMISTRY )
( 73) OH    + MGLY = XO2 + C2O3                 # 26000.           ;
( 74)         MGLY = C2O3 + HO2 + CO            # 0.021/L1         ;

  ( ISOPRENE CHEMISTRY )
( 75) O     + ISOP = 0.6*HO2 + 0.80*RCHO + 0.55*OLE + 0.50*XO2
                   + 0.50*CO + 0.45*ETH + 0.9*PAR
                                                # 27000.           ;
( 76) OH    + ISOP = XO2 + HCHO(+ 0.05*PAR) + 0.67*HO2 + 0.13*XO2N
                   + 1.0*ETH + 0.4*MGLY + 0.2*C2O3 + 0.2*RCHO
                                                # 142000.          ;
( 77) O3    + ISOP = HCHO + 0.4*RCHO + 0.55*ETH + 0.2*MGLY
                   + 0.10*PAR + 0.06*CO + 0.44*HO2 +0.1*OH
                                                # 0.018            ;
( 78) NO3   + ISOP = XO2N                       # 470.             ;

  (OPERATOR CHEMISTRY)
( 79) XO2   + NO   = NO2                        # 12000.0          ;
( 80) XO2   + XO2  =                            # 25.5      @ 1300.;
( 81) XO2N + NO    = (NTR)                      # 1000.0           ;
```

California Institute of Technology Mechanism

CIT has evolved from the Falls and Seinfeld mechanism and was put into its present form by McRae et al. [1982]. It uses a generalized species approach to represent hydrocarbon species and their chemistry. The rates of reaction of the generalized hydrocarbon species are mole weighted averages which depend on the initial concentrations of the hydrocarbons present. CIT was included in the evaluation with the intention of critiquing the current methanol impact assessment of Russell and Harris [1988b]. Russell was unable to directly provide a listing of the mechanism he was using for his work, but he referred me to the listings in Russell et al. [1988a] and Milford [1988]. These listings were used to compile the listing used in the chamber simulations, given in Table 2-5. This version differs from that given in Russel et al. [1988a] in the following ways: (1) The photolytic reaction rates are those calculated by Jeffries et al. [1988c]. (2) The rate of reaction 2 has been calculated assuming [O2]=210,000 ppm and [M]=1,000,000 ppm. (3) Reaction 35 is assumed to occur at the same rate as reaction 10. (4) Reaction 50 was divided into two reactions to simplify the rate expression. (5) Reaction 58 was omitted because ammonia was not present in any of the selected experiments.

In Russell et al. [1988a], the coefficient of RCHO in reaction 34 is 1.

$$RO \quad = \quad HO2 + 0.5*HCHO + RCHO \qquad (34)$$

In other reactions, RCHO becomes RO2 which becomes RO; thus, one and a half carbons, one in RCHO and a half in HCHO, are created without any loss in carbon from RO. In other listings of the mechanism [Milford, 1988; McRae et al., 1982], the coefficient of RCHO is given as 0.5. Because it was unclear which coefficient Russell and Harris [1988b] were using, I conducted the chamber simulations both ways. CIT-1 has a coefficient of 1 for RCHO in reaction 34, and CIT-2 has a coefficient of 0.5 for RCHO in reaction 34.

Russell et al. [1988a] do not specify the initial concentrations of hydrocarbons or reaction rates which were used to calculate the mole weighted average reaction rates for the generalized species in the mechanism. While McRae et al. [1982] provide example calculations of the generalized reaction rates, they do not provide the reaction rates for enough of the individual species to allow one to calculate the generalized rates for a different mixture. I assumed that the generalized rates used by Russell and Harris [1988b] assumed a fixed hydrocarbon mixture characteristic of the Los Angeles area. If this is true, then there is no reason to expect the mechanism to predict accurately with a mixture which is very different from this assumed mixture. For this reason, the evaluation of CIT-1 and CIT-2 has been limited to the experiments which use the SynUrban mixture.

TABLE 2-5: CIT Mechanism

```
CIT Chamber Mechanism
(******************************************************************
*****
Compiled from Russell, McCue, and Cass (1988) Environmental Science
and Technology, 22:263-271.

Photolytic rates are the same as CALL and CB4.  /E1 and /E2 denote
multiplication by 1/T and 1/T2, respectively.
*******************************************************************
****)
(1)  NO2            = NO  + O(3P)                 # 1.0/L1;
(2)  O(3P + O2 +M)  = O3  (+ M)                   # 7.27E+10 @
510/E2;
(Rate of above assumes [O2]=210000ppm and [M]=E+6ppm.)
(3)  O3   + NO      = NO2 (+ O2)                  # 1.04E+6 @-
1450/E1;
(4)  NO2  + O(3P)   = NO  (+ O2)                  # 3.99E+6/E1;
(5)  NO   + O(3P)   = NO2                         # 1.67E+5 @
584/E1;
(6)  NO2  + O(3P)   = NO3                         # 1.07E+6/E1;
(7)  NO2  + O3      = NO3 (+ O2)                  # 5.19E+4 @-
2450/E1;
(8)  NO3  + NO      = 2.*NO2                      # 8.05E+6/E1;
(9)  OH   + NO      = HONO                        # 5.07E+6/E1;
(10) HONO           = OH  + NO                    # 0.171/L1;
(11) HO2  + NO2     = HONO (+ O2)                 # 17.3 @ 1006/E1;
(12) OH   + HONO    = NO2 (+ H2O)                 # 2.91E+6/E1;
(13) HO2  + NO2     = HNO4                        # 1.73E+4
                                                          @1006/E1;
(14) HNO4           = HO2 + NO2                   # 1.80E+15
                                                          @-9950;
(15) HO2  + NO      = NO2 + OH                    # 3.58E+6/E1;
(16) NO   + RO2     = NO2  + RO                   # 3.58E+6/E1;
(17) NO2  + RCO3    = NO2 + RO2  (+ CO2)          # 3.36E+6/E1;
(18) OH   + NO2     = HNO3                        # 4.53E+6/E1;
(19) CO   + OH (+O2)= HO2 (+ CO2)                 # 1.31E+5/E1;
(20) O3             = O(3P + O2)                  # 0.001/L6;
(21) HCHO (+ 2O2)   = 2.*HO2 + CO                 # 0.001/L2;
(22) HCHO           = CO  (+ H2)                  # 0.001/L3;
(23) HCHO + OH (+O2)= HO2 + CO  (+ H2O)           # 1.50E+4;
(24) RCHO           = RO2 + HO2  + CO             # 0.0023/L5;
(25) RCHO + OH (+O2)= RCO3  (+ H2O)               # 2.36E+4;
(26) ETH  + OH      = RO2                         # 1.20E+4;
(27) ETH  + O(3P)   = RO2 + HO2                   # 1.219E+3;
(28) OLE  + OH      = RO2                         # 8.9142E+4;
(29) OLE  + O(3P)   = RO2 + RCO3                  # 2.2118E+4;
(30) OLE  + O3      = 0.5*RCHO + 0.5*HCHO + 0.3*HO2 +
                      0.31*RO2 + 0.14*OH + 0.03*RO
                                                  # 1.36E-1;
(31) ALK  + OH      = RO2                         # 5.80E+3;
(32) ALK  + O(3P)   = RO2 + OH                    # 99.8;
(33) AROM + OH      = RO2 + RCHO                  # 1.0112E+4;
(34) RO             = HO2 + 0.5*HCHO + RCHO       # 2.0E+5;
```

```
(35) RONO               = RO   + NO                 # 0.171/L1:
(The reaction above is assumed to occur at the same rate as
reaction 10.)
(36) NO    + RO         = RONO                      # 4.38E+6/E1;
(37) NO2   + RO         = RNO3                      # 2.19E+6/E1;
(38) NO2   + RO         = RCHO + HONO               # 1.91E+5/E1;
(39) NO2   + RO2        = RNO4                      # 1.64E+6/E1;
(40) H2O2 + OH          = HO2 (+ H2O)               # 2.50E+3;
(This reaction is different from the one listed in Milford (1987)
which is as follows:
(40) NO2   + RO2        = RCHO + HNO3               # 0;)

(41) RNO4               = NO2 + RO2                 # 1.80E+15@-9950;
(42) RCO3 + NO2         = PAN                       # 2.05E+6/E1;
(43) PAN                = NO2 + RCO3                # 4.77E+16
                                                          @-12516 ;
(44) NO2   + NO3        = N2O5                      # 7.40E+5/E1;
(45) N2O5               = NO3 + NO2                 # 4.06E+16
                                                          @-11080 ;
(46) N2O5 (+ H2O)       = 2.*HNO3                   # 5.66E-4/E1/W:
(47) OH    + O3         = HO2 (+ O2)                # 6.62E+5
                                                          @-1000/E1;
(48) HO2   + O3         = OH   (+ 2*O2)             # 4.85E+3
                                                          @-580/E1;
(49) (This reaction number was skipped in Russell, et al.)
(50a)HO2   + HO2        = H2O2 (+ O2)               # 2.5E+4
                                                          @ 1150/E1;
(50b)HO2   + HO2        = H2O2 (+ O2)               # 5.8E-5
                                                        @ 5800/W/E2;
(51) H2O2               = 2.*OH                     # 0.293E-3/L2;
(52) RO2 + RO2          = 2.*RO (+ O2)              # 2.04E+4
                                                          @ 223/E1;
(53) NO3 + HCHO(+O2)= HNO3 + HO2 + CO               # 0.43;
(54) NO3 + RCHO(+O2)= HNO3 + RCO3                   # 1.98;
(55) NO3                = NO2   + O(3P)             # 0.385/L6;
(56) NO3 + OLE          = RPN                       # 1826.7/E1;
(57) NO2 + NO3          = NO2   + NO (+ O2)         # 5.9E-1;

(OMIT..
(58) HNO3 + NH3         = NH4NO3;
     Ammonia was not used as an emission in any of the chamber
experiments.
... END OF OMIT)
```

Methanol Chemistry

It is generally agreed that the fate of methanol can be summarized by its reaction with an OH radical to form formaldehyde and a HO_2 radical [Ballentine et al., 1985]. This reaction was added to all of the mechanisms as it is given in Table 2-6.

To determine whether methyl nitrite has a significant effect on the predictions of the mechanisms, the photolysis of methyl nitrite to formaldehyde, nitric oxide, and a HO_2 radical has been included in the mechanisms as it is given in Table 2-6. The rate of this reaction is assumed to be equal to the photolysis of HONO.. The four chamber experiments which included methyl nitrite in the initial hydrocarbon mixture were simulated twice with both CB4 and CAL. For the first simulation, the methyl nitrite was considered to be part of the initial methanol concentration. In the second simulation, the methyl nitrite was explicitly represented as MEONO.

Chamber Effects Chemistry

Several reactions, shown in Table 2-6, were included in each mechanism to account for processes which occur in the chamber which are not significant in the atmosphere. The first of these reactions is the dark formation of nitrous and nitric acids produced by the reaction of NO_2 with water on the chamber walls [Jeffries and Sexton, 1985a]. This is the same reaction which was deleted from the listing of CAL above. The second reaction accounts for an ozone decay observed in the UNC chamber [Jeffries et al., 1982]. The rate used for this reaction in the chamber simulations was 1.8×10^{-5}, which is an order of magnitude less than the value recommended by Jeffries et al. [1982]. This discrepancy, however, has no significant effect on the predicted ozone profiles. The third reaction accounts for the background level of carbon monoxide and ozone that is brought in with the dilution air. The coefficients and rate are derived from measurements conducted at the UNC chamber site and estimations of the composition of continental background air [Jeffries and Sexton, 1985a].

Jeffries and Sexton [1985a] observed a source of NO_2 in the UNC chamber capable of producing 0.1 ppm of ozone during a 12 hour experiment. They suggested that the source of this nitrogen was nitrates which had been deposited on the walls during previous experiments. They also observed a source of radicals capable of making a significant contribution to the ozone production, which they attributed to a combination of the background air used to fill and dilute the chamber and the retention of substances, such as formaldehyde, on the chamber walls during previous experiments. After comparing several representations of these processes, Jeffries et al. [1988a] adopted a set of reactions recommended by Carter as the standard wall model for the UNC chamber. While simulating some experiments may require additional contributions from the walls and other experiments may require less, this set of reactions performs well on the average. OH radicals and NO_2 are produced in Carter's wall model at a rate proportional to light intensity. The conversion of OH to HO_2, which is supposedly due to background organic compounds, is represented by a simple first order reaction. These reactions were added to all the mechanisms as they are listed in Table 2-6.

To demonstrate the effect of the wall model on the performance of the rest of the mechanism, several simulations were repeated twice: once with a different wall model and once with no wall model. For this comparison, four experiments were selected a priori as representative of the mixtures in this study. In the second wall model, recommended by Killus [Jeffries et al., 1988a], the nitrogen and radical sources are represented as HONO and HCHO, which are produced at rates proportional to light intensity. The conversion of OH to HO_2 is indirectly represented by accounting for organic compounds brought in with the dilution air. For the comparison, these reactions were added, as they are listed in Table 2-6, to CAL and CB4 in place of the Carter model. I refer to these versions of the mechanisms as CAL-K and CB4-K. The same simulations were repeated again with the CAL and CB4 mechanisms without either of the wall reaction models. To signify no wall model, I refer to these versions of the mechanisms as CAL-N and CB4-N.

TABLE 2-6: Additional Reactions Added to the Mechanisms

```
( METHANOL CHEMISTRY )
     MEOH + OH    = HCHO + HO2                  # 1.98E+04@ -805.;

( METHYL NITRITE CHEMISTRY )
     MEONO        = HCHO + HO2 + NO             # 0.171/L1;

( CHAMBER EFFECTS REACTIONS )

   ( Mechanism Independent Reactions )
    NO2           = 0.21*HONO + 0.79*HNO3       # 1.6E-4;
    O3            =                             # 1.8E-5;
   ( Entrained with Dilution Air )
                  = 0.50*CO    + 0.70*O3        # 1.0/D;

   ( Carter's Wall Model )
    OH            = HO2                         # 250.0;
                  = OH                          # 0.30E-3/L1;
                  = NO2                         # 0.110E-3/L1;

   ( Killus' Wall Model )
   (Background HC brought in with dilution air
      ... 0.038 ppmC NMOC)
                  = 0.005*HCHO + 0.0025*ALD2 + 0.00062*ALK4 +
                    0.001*ETHE + 0.0005*PRPE + 0.0008*TOLU
                                                # 1.0/D;
                  = HONO                        # 0.11E-3/L1;
                  = HCHO                        # 0.22E-3/L1;
```

Speciation of Initial Hydrocarbons

Although the general concepts of the lumping schemes of the selected mechanisms were discussed in Part 1, it might not be clear from this general discussion how specific compounds were speciated. Table 2-7 lists all the compounds present in the SynAuto and SynUrban mixtures and the species used to represent them in the selected mechanisms. To account for HONO formation during the injection process, the initial concentration of HONO has been estimated as 7% of the initial NO_2 [Jeffries et al., 1988a].

TABLE 2-7: Mechanism Speciation for all Hydrocarbons in the Chamber Experiments

Compound	CIT	CAL	CB4
n-butane	ALK	ALK4	4 PAR
n-pentane	ALK	ALK7	5 PAR
isopentane	ALK	ALK4	5 PAR
2-methylpentane	ALK	ALK7	6 PAR
2,4-dimethylpentane	ALK	ALK7	7 PAR
2,2,4-trimethylpentane	ALK	ALK7	8 PAR
ethylene	ETH	ETHE	1 ETH
propylene	OLE	PRPE	1 PAR + 1 OLE
1-butene	OLE	PRPE	2 PAR + 1 OLE
trans-2-butene	OLE	TBUT	2 ALD2
cis-2-butene	OLE	TBUT	2 ALD2
2-methyl-1-butene	OLE	PRPE	3 PAR + 1 OLE
2-methyl-2-butene	OLE	TBUT	3 PAR + 1 ALD2
benzene	AROM	0.3 ALK7	1 PAR
toluene	AROM	TOLU	1 TOL
m-xylene	AROM	XYLE	1 XYL
o-xylene	AROM	XYLE	1 XYL
1,2,4-trimethylbenzene	AROM	TMBZ	1 PAR + 1 XYL
formaldehyde	HCHO	HCHO	1 HCHO

The Simulation Program

The chamber simulations for this evaluation were conducted using the Photochemical Kinetics Simulation System (PC-PKSS) developed by Jeffries [1987a]. The system is a collection of computer programs which converts a list of photochemical reactions, the mechanism, to a system of coupled differential equations. Using input tables of initial concentrations and time dependent conditions, such as light, temperature, humidity, and dilution, the programs solve the system of equations to yield concentrations of species as functions of time.

Given the species concentrations and conditions at a time t, the programs calculate the rate of each reaction in the mechanism. For each species in a reaction, the rate is multiplied by the stoichiometric coefficient of the species and assigned a sign according to whether the species was a reactant or a product. The rates of all reactions affecting a species are summed to yield a derivative for the species concentration at time t. By numerically integrating this derivative over a small time step h, the programs calculate the species concentration at time t+h. This process is repeated between 80 and 200 times in a chamber simulation [Jeffries, 1984].

To demonstrate the correct implementation and solution of the mechanisms, test simulations were compared to the example simulations provided by the mechanism developers.

The implementation of CAL was tested using Test Problem 1 from Lurmann et al. [1987]. The CAL mechanism was modified for the test case to account for the constant solar radiation conditions specified in Table 2-15 [Lurmann et al., 1987]. The agreement between the PC-PKSS/CAL predictions and the values given by Lurmann et al. is shown in Figure 2-1.

The documentation for CB4 does not contain a simple test case, but the inputs and outputs of example chamber simulations were obtained on magnetic disk from Gery [1988]. After CB4 was modified to agree with Gery's representation of the wall process, the PC-PKSS/CB4 predictions agreed with the Gery's predictions, as shown in Figures 2-2 and 2-3.

The original references for the CIT mechanism do not contain a test case, and Russell and Harris were not able to provide me with an example from the mechanism that they are using. The only example simulations available for the CIT mechanism are three simulations completed by Milford [1988]. Of the three simulations, I was only able to reasonably duplicate one, as is seen in Figures 2-4, 2-5, and 2-6. In trying to duplicate these simulations, however, I discovered several typographical errors in the mechanism listing and initial conditions in Milford [1988]. Because of these errors, I do not regard these simulations as adequate test cases. However, the failure to duplicate two of the simulations may be due to an error in my implementation of the mechanism; therefore, all conclusions of this evaluation regarding the performance of the CIT mechanism should be considered suspect.

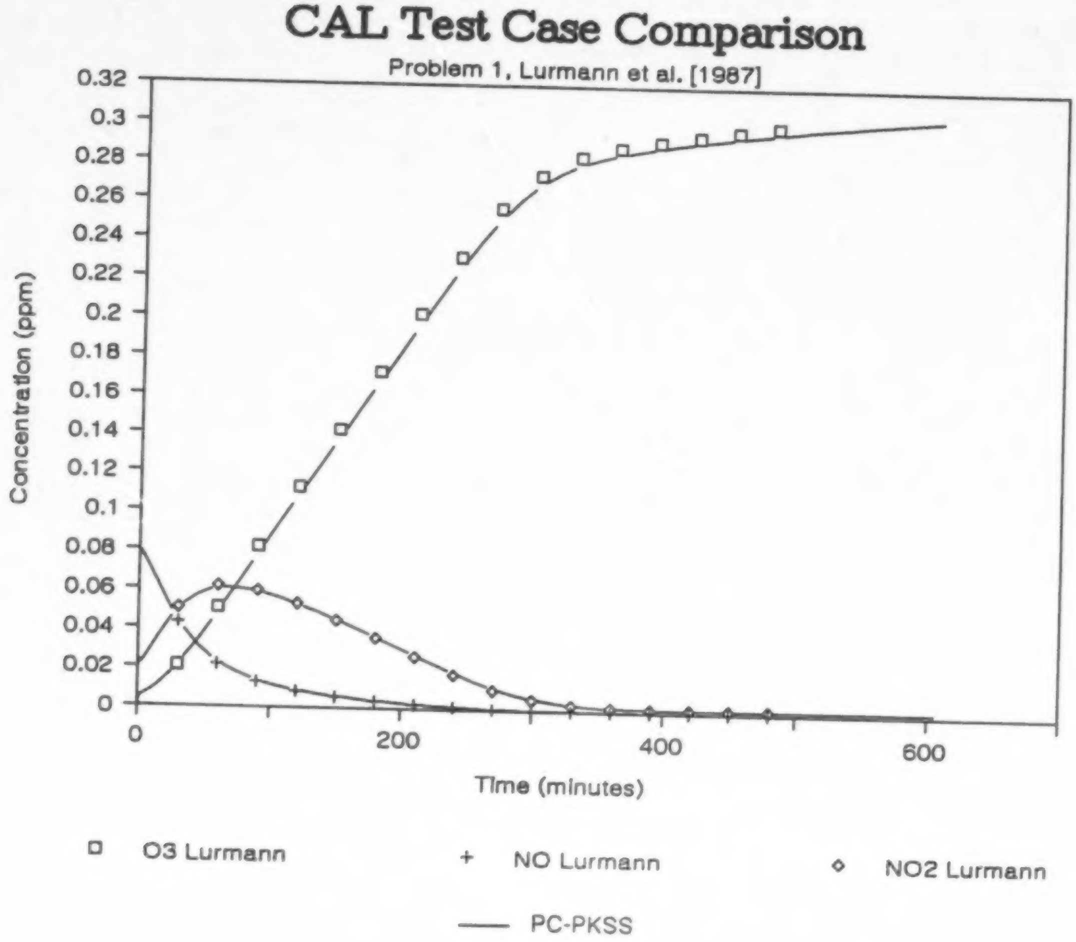


Figure 2-1. CAL Test Case Comparison.

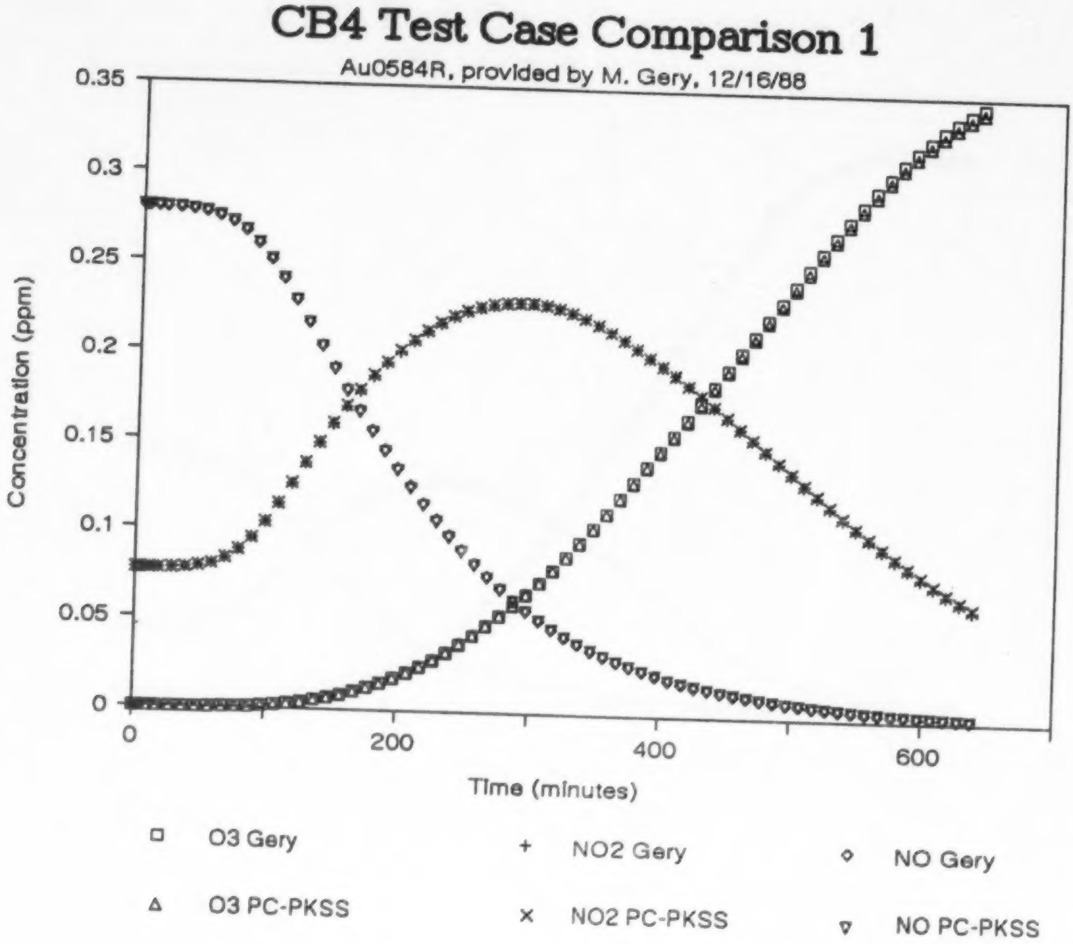


Figure 2-2. CB4 Test Case Comparison 1.

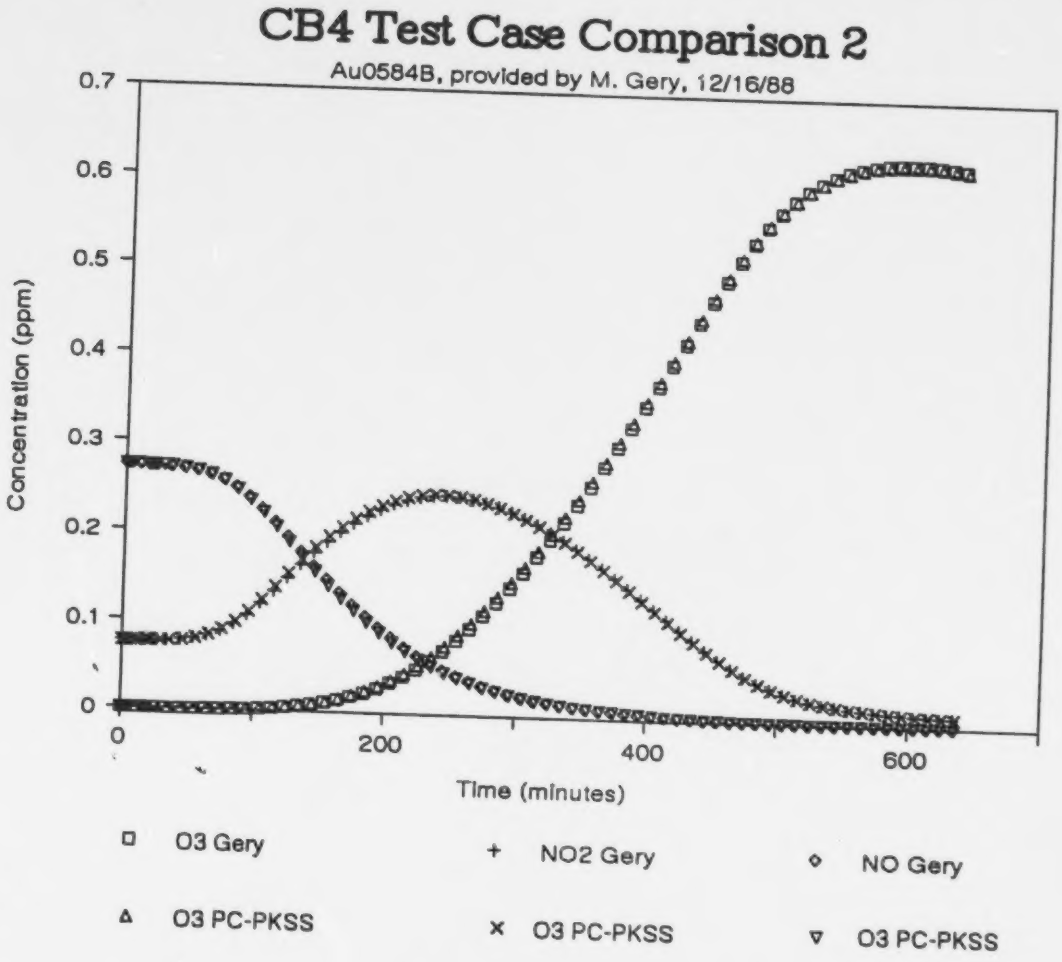


Figure 2-3. CB4 Test Case Comparison 2.

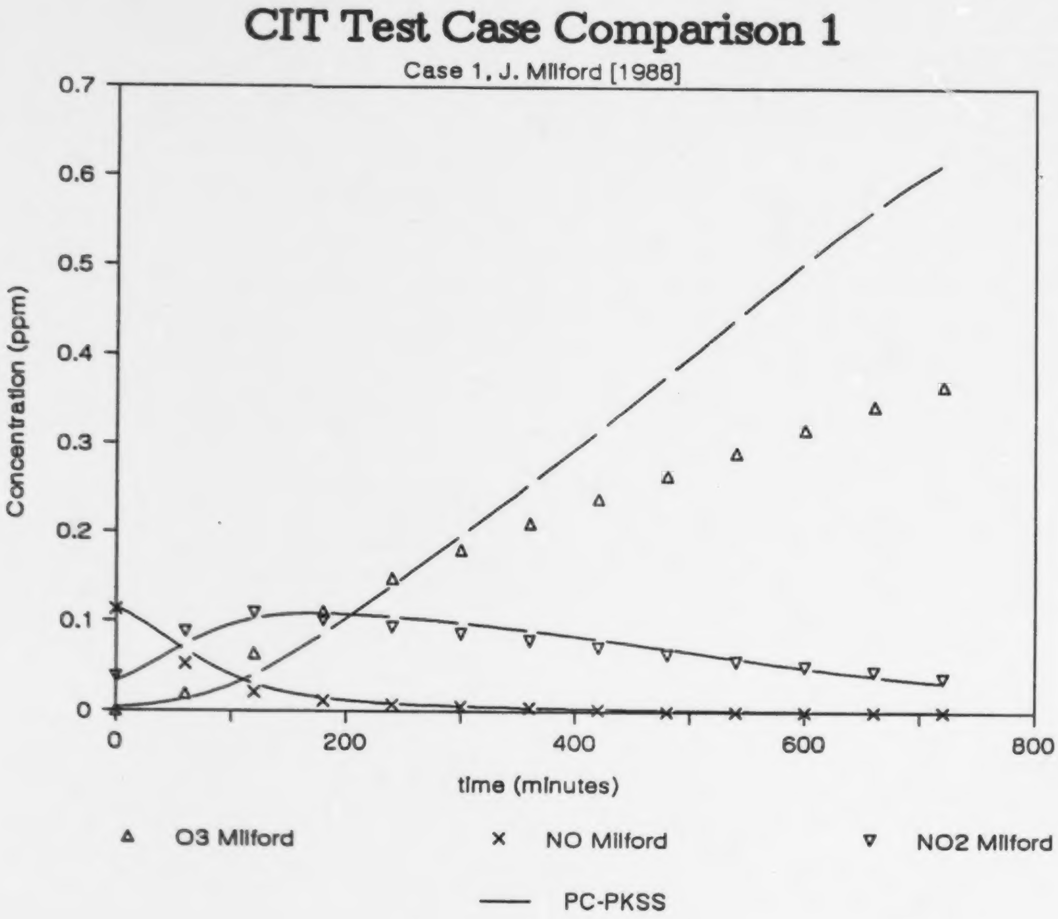


Figure 2-4. CIT Test Case Comparison 1.

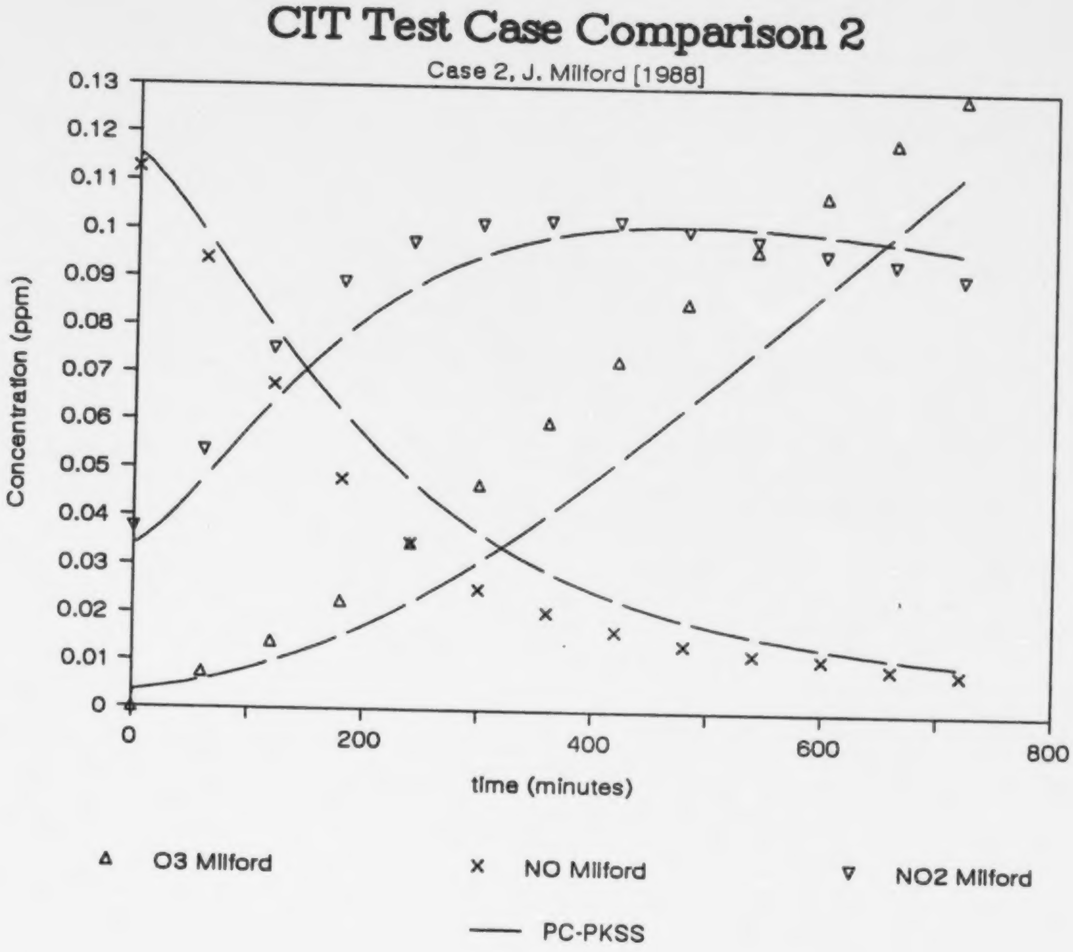


Figure 2-5. CIT Test Case Comparison 2.

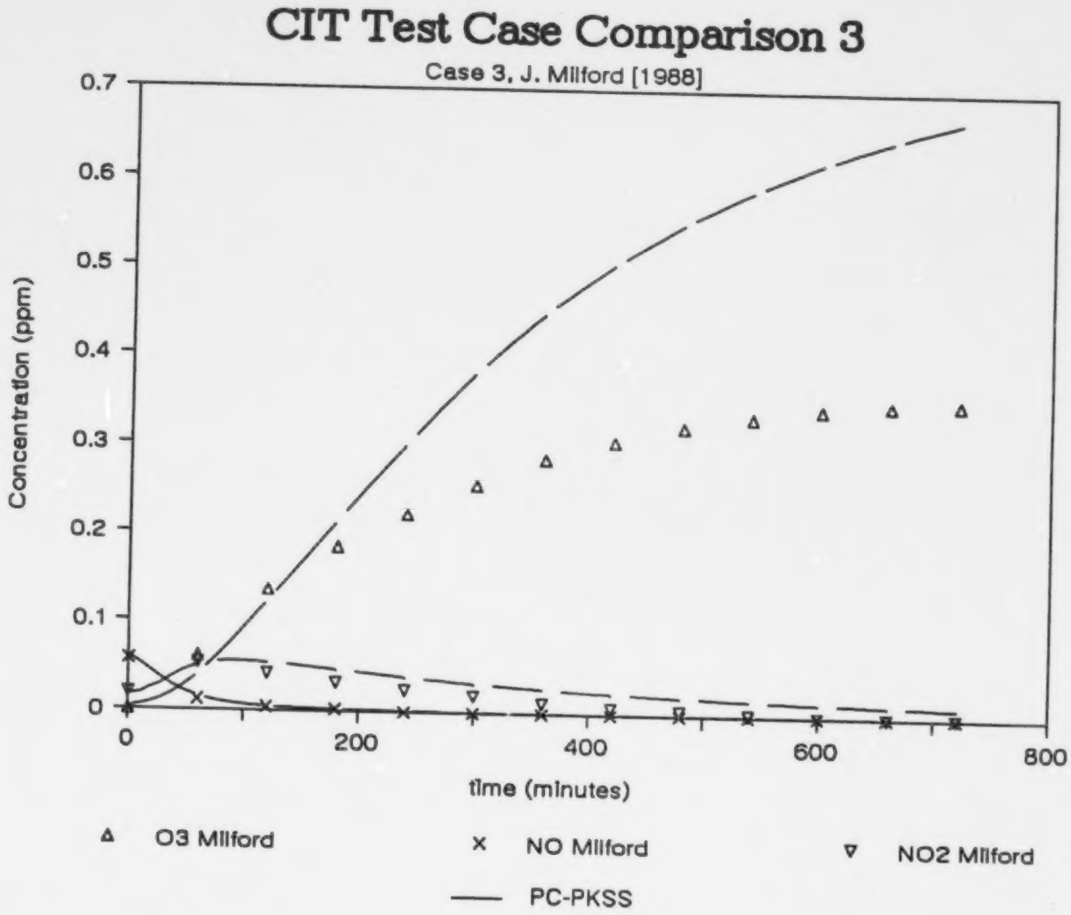


Figure 2-6. CIT Test Case Comparsion 3.

Uncertainty and Agreement

The predictions of a model may not agree with the observations from a chamber experiment for several reasons: (1) The chemical mechanism may not correctly represent the gas phase chemistry occuring in the chamber. (2) The effects of the chamber, including light characteristics, wall processes, and background air, may not be represented adequately in the model. (3) The initial conditions of the experiment may not be correctly specified in the model. (4) The mathematical solution or implementation of the model may be flawed. (5) The measurements of the species concentrations in the chamber may not be accurate.

To evaluate the correctness of the model, the other uncertainties must be understood. Ideally, one could quantify all the sources of uncertainty in the chamber observations and then calculate confidence limits for the observed concentrations. One could also quantify all the sources of uncertainty in the model input conditions and chamber characterizations and then generate a series of prediction plots which define confidence limits within which model predictions could be expected given the input uncertainty. As discussed by Dunker [1987], the areas in which the confidence limits of the observational data and the confidence limits of the model predictions over lapped would constitute reasonable agreement. See Figure 2-7. In reality, however, many uncertainties cannot be quantified.

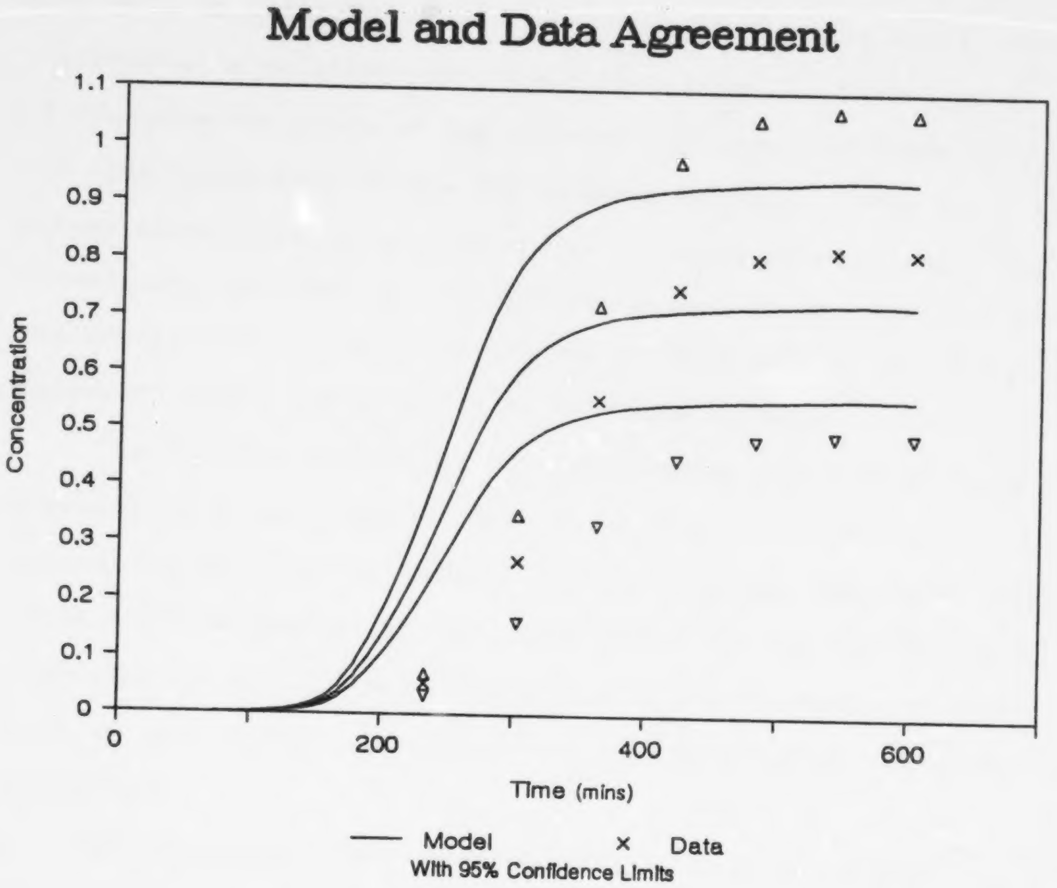


Figure 2-7. Model and Data agreement.

The uncertainty in the characterization of the chamber is difficult to quantify. The light characterization model used in the chamber simulations was described above. Jeffries et al. [1988c] display plots of the modeled and observed light intensities for each experiment in the UNC chamber database. The light model agrees exceptionally well with the observed intensities. The uncertainty involved in the representation of the wall processes and background air is demonstrated in this work by using two different model representations of these effects.

The initial conditions for the chamber simulations were compiled from the computer data files for the experiments. The initial conditions for some of the experiments have been revised since the publication of the final report of the UNC methanol study [Jeffries et al., 1985b]. The actual initial condition files for each of the chamber simulations in this evaluation are shown in Appendix B.

The accuracy of the PC-PKSS program and the proper implementation of the mechanisms are demonstrated in the test cases presented above. Given that the utility of a model is dependent on its proper implementation, it is useful to compare the relative availability of guidance documentation for each of the mechanisms. Some important elements of mechanism documentation and their availability for CAL, CB4, and CIT are summarized in Table 2-8.

TABLE 2-8: Important Components of Mechanism Documentation and their Availability for CAL, CB4, and CIT

Important Components of Documentation	Availability CAL	 CB4	 CIT
list of reactions and species	X	X	X
rules for speciating common organic mixtures	X	X	X
dependence of rate constants on actinic flux	X	X	
dependence of rate constants on temperature, pressure, and hydrocarbon mixture	X	X	
identification of differences in reactions and rate constants for use in chambers vs. ambient air	X	X	
chamber test cases including input and output conditions	X		
ambient air test cases including input and output conditions	X	X	

Putting error bars around analytical measurements is difficult, but there are several ways that one can get an understanding of the level of accuracy and precision. By examining the calibration factors for an instrument over a long period of time, one can evaluate the precision of the instrument and its operator. The accuracy of an instrument can be evaluated by comparing its measurements of several different calibration sources or by comparing its measurements to those of other instruments of a different type.

Ozone

The developers of CB4 and CAL state that the mechanisms predictions of ozone maxima agree within 30% of the observed maxima in chamber experiments of complex mixtures [Jeffries et al., 1988a]. In the chamber experiments, the ozone concentration was measured continuously with a Bendix 8002 chemiluminescence monitor with a detection limit of 0.001 ppm and a range of 0 to 2 ppm. This instrument was calibrated twice daily using a UV-quartz ozone generator. The calibration factors for this instrument for the selected experiments had a standard deviation of 4%. The maximum difference between calibration factors on the same day was also 4% [Jeffries et al., 1985c]. These statistics, however, only reflect the precision of the instrument and not the accuracy.

The accuracy of the ozone measurements is affected by a reaction which occurs in the sample line running from the chamber to the instrument [Jeffries and Sexton, 1985a]. This reaction is only important when both NO and NO_2 concentrations are relatively high. Except under these conditions, the measurement error is considerably less than the 30% error expected in the models, and therefore, a difference between observed and predicted concentrations of 30% is accepted as reasonable agreement for ozone.

Formaldehyde

Formaldehyde concentrations were measured during the chamber experiments by a CEA 555, an automated colorimetric instrument which uses a reverse West-Gaeke technique. The instrument has a detection limit of 0.02 ppm. A positive interference has been observed in which 5% of the acetaldehyde present appears as formaldehyde when acetaldehyde is present at concentrations between 0.1 and 1 ppmV. Interferences from other carbonyls have not been observed. The baseline response of the instrument tends to drift upward over time requiring that a clock timer switch the inlet valve to a zero formaldehyde stream every 3 to 4 hours in order to establish a moving baseline. A failure of the timing clock would most likely result in an over reporting of the concentration. The instrument is also sensitive to the stability of the sample air flow, which usually drifts downward, resulting in an under reporting of the concentration [Jeffries et al., 1988a].

There were two calibration sources used during the selected experiments: liquid standards prepared by serial dilution of commercial 37% formaldehyde solution and batch standards prepared by subliming precision weighed quantities of 95% pure paraformaldehyde. The standard deviation of the calibration factors for the entire 1984 season was 33%, and the largest difference between two calibration factors obtained on the same day was 31% [Jeffries et al., 1985c]. The majority of the formaldehyde calibrations, however, took place during the start or finish of the experimental season; therefore, these statistics are not necessarily representative of the period during which the experiments were conducted.

In the summer of 1986, a formaldehyde measurement comparison study was conducted in the UNC chamber [Jeffries et al., 1988a]. Five different analytical methods were used to measure formaldehyde concentrations, and there was never more than a 10% difference between the measurements of the CEA instrument and the group mean measurement of the other intstruments. During this study, the CEA instrument was calibrated with the two sources described above and a commercial permeation tube system. The calibration factors from the study period for all three sources had a standard deviation of 8.6%. The factors for the liquid standards only had a standard deviation of 9.2%; the factors for the chamber injections of paraformaldehyde had a standard deviation of 6.4%; and the permeation tube factors had a standard deviation of 5.3%.

Given the precision and apparent accuracy of the CEA instrument during the comparison study, I believe that the variability observed in the calibration factors for the beginning and end of the 1984 season are representative of the worst case. While the uncertainty in the UNC formaldehyde measurements is probably never better than 5%, it is probably never worse than about 30%. Therefore, I define reasonable agreement between formaldehyde observations and predictions as being within 30% of the observed concentrations.

PAN

PAN concentrations in the chamber were measured by a gas chromatograph using electron capture detection. This instrument was calibrated by comparing its response to the response of a calibrated chemiluminescent NO_2 monitor for a pure sample of PAN. The chemiluminescent monitor reports 100% of the PAN as NO_2 [Jeffries et. al., 1985a]. The NO_2 concentration profiles that are given in Appendix A for the chamber experiments have not been corrected for this simultaneous measurement of PAN. At the end of an experiment, most of what is reported as NO_2 is actually PAN, and therefore, one should expect that the mechanism predictions of NO_2 will be lower than the reported chamber observations. At the same time, the mechanism predictions or chromatographic measurements of PAN should not exceed the reported concentration of NO_2. The uncertainty in the chromatographic PAN measurements is believed to be on the same order as the uncertainties for ozone and formaldehyde. Thus, I define reasonable agreement between PAN observations and predictions as being within 30% of the observed concentrations.

Evaluating Model Performance

Having defined reasonable agreement, one can begin to evaluate the level of agreement between model predictions and chamber observations. This evaluation process takes the form of a series of questions, or determinations, which provide explanations, other than the incorrectness of the mechanism, for observed disagreements. If no reasonable explanation, such as the uncertainties described above, can be found, then it is assumed that the mechanism incorrectly represents the gas phase chemistry occuring in the chamber.

The series of questions begins by determining whether the proper initial species concentrations were established for the simulation. In the initial minutes of the experiments, some of the chamber measurements have a great deal of variation due to mixing and instrument sensitivity. This variation must be accounted for when determining the true initial concentration.

If the initial concentrations used in the simulation agree with those measured in the experiment, then one can check the adequacy of the representation of the background and wall species. The timing of the point at which the concentrations of NO and NO_2 are equal, referred to as the NO_x crossover point, is an indication of the initial population of radicals. Until this point is reached, the chemistry is dominated by inorganic reactions which have been well described and are thought to be accurately represented in the mechanisms. If the mechanisms fail to properly predict the timing of the crossover, then one can assume that it is due to an inaccurate representation of the chamber effects.

If the predicted crossover is later than the observed crossover, there may be a source of radicals present in the chamber which is not represented in the mechanism. One source of these radicals may be condensed water on the walls of the chamber which has adsorbed nitrogenous species during previous experiments. As the water evaporates, the nitrogen is returned to the gas phase as HONO. The presence of condensed water can be confirmed by comparing the chamber temperature and dewpoint during the morning hours of the experiment. Gery [1988] has demonstrated that for experiments which have a morning temperature which falls below the dewpoint, the NO_x crossover point can be correctly modeled by slowly adding a finite amount of HONO as the temperature increases.

If the predicted crossover is earlier than the observed crossover, the magnitude of wall processes, represented explicitly in a specified wall model or implicitly in the gas phase chemistry itself, may be overestimated.

The relative timing established by the model predictions of the NO_x crossover point should be carried all the way through the simulation. If misrepresentation of the background and wall processes leads to a late crossover prediction, the maximum predicted ozone concentration would also be expected to be late compared to the observed ozone maximum. In this case, if the timing of the predicted ozone maximum agreed with the timing of the observed ozone maximum, then the mechanism is too reactive in the formation of ozone. The failure to represent the initial population of radicals should not significantly affect the timing of the subsequent gas phase chemistry predicted by the mechanism.

The accuracy of the subsequent production of radicals is determined by examining the slopes of the predicted and observed hydrocarbon decay profiles. If the predicted decay is steeper than the observed decay, then the mechanism is producing too many radicals and would be expected to over predict the maximum ozone concentration. If the predicted decay is less steep than the observed decay, then the mechanism is not producing enough radicals and would be expected to under predict the maximum ozone concentration.

If the predicted hydrocarbon decay profiles are correct, then the ozone predictions should agree with the observed concentrations. The predicted concentration profiles for formaldehyde and PAN should also agree with the chamber observations.

This evaluation process was conducted for each of the simulations and is presented in Appendix A. For each chamber experiment, the appendix contains a discussion of the performance of the various mechanisms and plots of the model predictions and chamber observations.

A Summary of Model Performance

The results of the evaluation process were compiled and examined for patterns of model performance. Theoretically, the models should perform the same on the control side of the chamber for experiments using the same control mixture. The performance of the models on the substitution/ replacement side of the chamber may vary, but trends should be evident within experiments using the same control mixture. Such consistent patterns, however, did not always appear in the chamber simulations. Instead, the models performed similarly on both sides of the chamber for a given experiment regardless of the composition of the mixtures being modeled. This result suggests that model performance is more dependent on other experimental conditions than it is on the composition of the mixtures being modeled. Even with this result, however, some general trends can be recognized.

CAL and CB4 Predictions

Despite their differences in the representation of hydrocarbons, CAL and CB4 perform very similarly. This is not necessarily suprising given that the mechanisms were developed using the same chamber databases and kinetics literature. Tables 2-9, 2-10, and 2-11, summarize the performance of CAL and CB4.

TABLE 2-9: A Comparison of Observed and CAL and CB4 Predicted Ozone Concentrations

HC/NOx Ratio	Control Mixture	Reduction or Substitution	Date	Control Side		Treatment Side	
				CAL	CB4	CAL	CB4
9:1	SynAuto	1/3 HC reduction	Au0684	adequate	adequate	adequate	adequate
		1/3 MEOH w/20% HCHO	Au0884	adequate	adequate	adequate	adequate
	SynUrban	1/3 HC reduction	Jn2685	adequate	adequate	adequate	adequate
		1/3 MEOH w/ 0% HCHO	St0184	adequate	adequate	high	high
		1/3 MEOH w/20% HCHO	Au2284	adequate	adequate	adequate	adequate
3:1	SynAuto	1/3 HC reduction	Au0584	adequate	adequate	adequate	adequate
		1/3 MEOH w/ 0% HCHO	Au0784	adequate	adequate	adequate	adequate
		1/3 MEOH w/10% HCHO	Au0484	adequate	adequate	high	high
		1/3 MEOH w/20% HCHO	Au0984	adequate	adequate	adequate	adequate
	SynUrban	1/3 HC reduction	St0284	very high	very high	very high	very high
		1/3 MEOH w/10% HCHO	Au2584	high	high	high	high
		1/3 MEOH w/10% HCHO	Jn2885	very high	very high	very high	very high
		1/3 MEOH w/20% HCHO	St0384	very high	very high	very high	very high
9:1	SynAutoUrban	1/3 HC reduction	St0884	adequate	adequate	adequate	adequate
		1/3 MEOH w/10% HCHO	St1784	adequate	adequate	adequate	adequate
		HCHO addition	St2184	adequate	adequate	adequate	adequate
	HMWMIX	1/3 HC reduction	St1984	adequate	adequate	adequate	adequate

Note: "Adequate" indicates that model predictions and observed data were within 30% of one another. "High" and "very high" indicate that the model over predicts the observed data by more than 30% and 100%, respectively. "Low" and "very low" indicate that the model under predicts the observed data by more than 30% and 50%, respectively.

TABLE 2-10: A Comparison of Observed and CAL and CB4 Predicted Formaldehyde Concentrations

HC/NOx Ratio	Control Mixture	Reduction or Substitution	Date	Control Side		Treatment Side	
				CAL	CB4	CAL	CB4
9:1	SynAuto	1/3 HC reduction	Au0684	high	high	adequate	adequate
		1/3 MEOH w/20% HCHO	Au0884	adequate	adequate	adequate	adequate
	SynUrban	1/3 HC reduction	Jn2685	very low	very low	very low	very low
		1/3 MEOH w/ 0% HCHO	St0184	adequate	adequate	adequate	adequate
		1/3 MEOH w/20% HCHO	Au2284	low	low	low	low
3:1	SynAuto	1/3 HC reduction	Au0584	adequate	adequate	adequate	adequate
		1/3 MEOH w/ 0% HCHO	Au0784	adequate	adequate	adequate	adequate
		1/3 MEOH w/10% HCHO	Au0484	very high	very high	very high	very high
		1/3 MEOH w/20% HCHO	Au0984	low	low	low	low
	SynUrban	1/3 HC reduction	St0284	low	low	very low	very low
		1/3 MEOH w/10% HCHO	Au2584	low	low	low	low
		1/3 MEOH w/10% HCHO	Jn2885	adequate	adequate	low	low
		1/3 MEOH w/20% HCHO	St0384	adequate	adequate	adequate	adequate
9:1	SynAutoUrban	1/3 HC reduction	St0884	?	?	?	?
		1/3 MEOH w/10% HCHO	St1784	low	low	adequate	adequate
		HCHO addition	St2184	adequate	adequate	adequate	adequate
	HMWMIX	1/3 HC reduction	St1984	low	low	low	low

Note: "Adequate" indicates that model predictions and observed data were within 30% of one another. "High" and "very high" indicate that the model over predicts the observed data by more than 30% and 100%, respectively. "Low" and "very low" indicate that the model under predicts the observed data by more than 30% and 50%, respectively.

TABLE 2-11: A Comparison of Observed and CAL and CB4 Predicted PAN Concentrations

HC/NOx Ratio	Control Mixture	Reduction or Substitution	Date	Control Side		Treatment Side	
				CAL	CB4	CAL	CB4
9:1	SynAuto	1/3 HC reduction	Au0684	?	?	?	?
		1/3 MEOH w/20% HCHO	Au0884	high	adequate	high	high
	SynUrban	1/3 HC reduction	Jn2685	very high	very high	very high	very high
		1/3 MEOH w/ 0% HCHO	St0184	very high	very high	very high	very high
		1/3 MEOH w/20% HCHO	Au2284	?	?	?	?
3:1	SynAuto	1/3 HC reduction	Au0584	very high	high	very high	adequate
		1/3 MEOH w/ 0% HCHO	Au0784	very high	adequate	very high	adequate
		1/3 MEOH w/10% HCHO	Au0484	high	adequate	very high	adequate
		1/3 MEOH w/20% HCHO	Au0984	high	adequate	high	adequate
	SynUrban	1/3 HC reduction	St0284	high	adequate	adequate	low
		1/3 MEOH w/10% HCHO	Au2584	very high	very high	very high	very high
		1/3 MEOH w/10% HCHO	Jn2885	very high	very high	very high	very high
		1/3 MEOH w/20% HCHO	St0384	?	?	?	?
9:1	SynAutoUrban	1/3 HC reduction	St0884	very high	very high	very high	very high
		1/3 MEOH w/10% HCHO	St1784	very high	very high	very high	very high
		HCHO addition	St2184	high	high	high	high
	HMWMIX	1/3 HC reduction	St1984	high	high	high	high

Note: "Adequate" indicates that model predictions and observed data were within 30% of one another. "High" and "very high" indicate that the model over predicts the observed data by more than 30% and 100%, respectively. "Low" and "very low" indicate that the model under predicts the observed data by more than 30% and 50%, respectively.

The ozone predictions of the mechanisms agree reasonably well with the observed concentrations in all of the experiments except the least reactive experiments involving SynUrban at a HC/NO_x ratio of 3:1. For these experiments, the mechanisms are generally too reactive and over predict the observed ozone concentrations by large margins.

CAL and CB4's abilities to predict formaldehyde concentrations are much less consistent. While there is no consistent trend for the experiments involving SynAuto, the SynUrban experiments show a relatively consistent pattern of under prediction. Increasing the formaldehyde emissions through methanol substitution has no effect on the performance of either mechanism.

The two mechanisms differ in their ability to predict PAN concentrations. CAL generally over predicts the observed PAN concentrations by significant margins. While CB4 also over predicts PAN concentrations for most of the experiments, it performs reasonably well for the SynAuto experiments at a HC/NO_x ratio of 3:1.

The ability of the mechanisms to predict the relative differences between species concentrations on the two sides of the chamber is summarized in Table 2-12. Both mechanisms tend to under predict the decreases in ozone concentrations due to hydrocarbon reduction or methanol substitution. Therefore, the mechanisms would tend to under predict the benefits of MFV programs as ozone control strategies.

TABLE 2-12: The Ability of CAL and CB4 to Predict Relative (Side-to-Side) Changes in Ozone Concentrations

HC/NOx Ratio	Control Mixture	Reduction or Substitution	Date	CAL & CB4
9:1	SynAuto	1/3 HC reduction	Au0684	adequate
		1/3 MEOH w/20% HCHO	Au0884	adequate
	SynUrban	1/3 HC reduction	Jn2685	under
		1/3 MEOH w/ 0% HCHO	St0184	under
		1/3 MEOH w/20% HCHO	Au2284	adequate
3:1	SynAuto	1/3 HC reduction	Au0584	adequate
		1/3 MEOH w/ 0% HCHO	Au0784	adequate
		1/3 MEOH w/10% HCHO	Au0484	under
		1/3 MEOH w/20% HCHO	Au0984	adequate
	SynUrban	1/3 HC reduction	St0284	under
		1/3 MEOH w/10% HCHO	Au2584	adequate
		1/3 MEOH w/10% HCHO	Jn2885	over
		1/3 MEOH w/20% HCHO	St0384	adequate
9:1	SynAutoUrban	1/3 HC reduction	St0884	under
		1/3 MEOH w/10% HCHO	St1784	adequate
		HCHO addition	St2184	under
	HMWMIX	1/3 HC reduction	St1984	adequate

Overall, CAL and CB4 predict concentrations of ozone quite well. Their ability to predict formaldehyde concentrations is not as good, and their ability to predict PAN concentrations is quite poor.

CIT Predictions

Varying the coefficients in CIT-1 and CIT-2 had a very interesting effect on the ability of the mechanism to predict different species. The performance of both versions is summarized in Tables 2-13, 2-14, and 2-15.

CIT-1 consistently over predicted the observed ozone concentrations by wide margins. The feedback loop created by the coefficient of 1 in reaction 34 drives the formation of ozone much too high. CIT-2, however, performs quite well until the end of the simulations. In the late afternoon when the formation of ozone typically slows down, CIT-2 continues to produce ozone at a constant rate resulting in an over prediction of the maximum ozone concentration. McRae et al. [1982] suggested that such a problem may occur due to the method used to calculate the rate constants for the generalized species in the mechanism. Because the most reactive compounds of a given class would be consumed first, a mole-weighted average rate constant actually under estimates the rates at the beginning of an experiment and over estimates the rates at the end. McRae et al. [1982] argue that this is not a problem in ambient modeling because hydrocarbons are continually emitted into the atmosphere.

While changing the coefficients in reaction 34 improves the ozone predictions, the change does not improve the formaldehyde predictions. As with CAL and CB4, the CIT mechanisms generally under predict the observed formaldehyde concentration profile. CIT-1 often performs better than CIT-2, but neither version duplicates the shape of the observed formaldehyde profile well.

The timing of the over prediction of ozone suggests that the mechanism does not properly represent the late afternoon formation of PAN and nitric acid either. As expected, neither CIT-1 or CIT-2 correctly predicts the observed concentration of PAN, although the margin of error is generally less than that produced by CB4 and CAL. While CB4 and CAL tend to over predict PAN concentrations, the CIT mechanisms tend to under predict the observed PAN concentrations.

In the test cases for CIT presented earlier, the predicted ozone concentrations were much greater than those reported by Milford [1988]. Therefore, it is unclear if the over prediction observed in the chamber simulations is due to an error in the implementation of the mechanism or an error in the mechanism itself.

TABLE 2-13: A Comparison of Observed and CIT-1 and CIT-2 Predicted Ozone Concentrations

HC/NOx Ratio	Control Mixture	Reduction or Substitution	Date	Control Side CIT-1	Control Side CIT-2	Treatment Side CIT-1	Treatment Side CIT-2
9:1	SynUrban	1/3 HC reduction	Jn2685	very high	high	very high	high
		1/3 MEOH w/ 0% HCHO	St0184	very high	high	very high	adequate
		1/3 MEOH w/20% HCHO	Au2284	very high	high	very high	high
3:1	SynUrban	1/3 HC reduction	St0284	very high	adequate	very high	high
		1/3 MEOH w/10% HCHO	Au2584	very high	adequate	very high	adequate
		1/3 MEOH w/10% HCHO	Jn2885	very high	adequate	very high	high
		1/3 MEOH w/20% HCHO	St0384	very high	high	very high	high

Note: "Adequate" indicates that model predictions and observed data were within 30% of one another. "High" and "very high" indicate that the model over predicts the observed data by more than 30% and 100%, respectively. "Low" and "very low" indicate that the model under predicts the observed data by more than 30% and 50%, respectively.

TABLE 2-14: A Comparison of Observed and CIT-1 and CIT-2 Predicted Formaldehyde Concentrations

HC/NOx Ratio	Control Mixture	Reduction or Substitution	Date	Control Side CIT-1	Control Side CIT-2	Treatment Side CIT-1	Treatment Side CIT-2
9:1	SynUrban	1/3 HC reduction	Jn2685	low	low	low	low
		1/3 MEOH w/ 0% HCHO	St0184	very high	adequate	very high	adequate
		1/3 MEOH w/20% HCHO	Au2284	low	low	low	low
3:1	SynUrban	1/3 HC reduction	St0284	low	low	very low	very low
		1/3 MEOH w/10% HCHO	Au2584	low	very low	low	very low
		1/3 MEOH w/10% HCHO	Jn2885	adequate	low	adequate	low
		1/3 MEOH w/20% HCHO	St0384	adequate	low	adequate	low

Note: "Adequate" indicates that model predictions and observed data were within 30% of one another. "High" and "very high" indicate that the model over predicts the observed data by more than 30% and 100%, respectively. "Low" and "very low" indicate that the model under predicts the observed data by more than 30% and 50%, respectively.

TABLE 2-15: A Comparison of Observed and CIT-1 and CIT-2 Predicted PAN Concentrations

HC/NOx Ratio	Control Mixture	Reduction or Substitution	Date	Control Side CIT-1	Control Side CIT-2	Treatment Side CIT-1	Treatment Side CIT-2
9:1	SynUrban	1/3 HC reduction	Jn2685	very low	very low	very low	very low
		1/3 MEOH w/ 0% HCHO	St0184	low	low	low	low
		1/3 MEOH w/20% HCHO	Au2284	?	?	?	?
3:1	SynUrban	1/3 HC reduction	St0284	low	low	low	low
		1/3 MEOH w/10% HCHO	Au2584	low	adequate	low	high
		1/3 MEOH w/10% HCHO	Jn2885	adequate	very low	adequate	very low
		1/3 MEOH w/20% HCHO	St0384	?	?	?	?

Note: "Adequate" indicates that model predictions and observed data were within 30% of one another. "High" and "very high" indicate that the model over predicts the observed data by more than 30% and 100%, respectively. "Low" and "very low" indicate that the model under predicts the observed data by more than 30% and 50%, respectively.

The Effect of Methyl Nitrite

The effect of explicitly representing methyl nitrite in the chamber simulations is summarized in Table 2-16. In all four of the experiments, the explicit representation affected only the formaldehyde concentration profile. By producing more formaldehyde sooner, the explicit representation improved the predictions of CAL and CB4 but only by a very small amount.

The impact of methyl nitrite may be masked by the fact that all of the species was injected into the chamber before dawn. If the methyl nitrite had been injected into the chamber in full daylight, the species' photodissociation may have had a more significant effect on the production of ozone and formaldehyde. Trajectory or airshed modeling is needed to conclusively evaluate this possibility.

The Effect of the Wall Model

Changing or eliminating the wall model had the same effect on the mechanism predictions for all four of the experiments selected for the comparison. CAL-K and CB4-K always produced less ozone and PAN and more formaldehyde than CAL and CB4 with Carter's wall model. CAL-N and CB4-N always produced less of all three species than with either wall model. Whether or not this change improved the performance of the mechanisms depended upon whether the mechanisms had originally over predicted or under predicted the observed concentrations. As shown in Table 2-17, no one representation of the wall process produced the best predictions for all three species in any of the four experiments. Carter's model, however, was not the best wall model for any of the species in any of the four experiments.

Quantitatively, the impact of the wall models on the predictions of the mechanisms in their entirety is varied and may be as little as 10% of the observed concentrations. The maximum difference between predictions with a wall model and without a wall model are about 200%, 100%, and 400% of the observed concentrations of ozone, formaldehyde, and PAN, respectively.

TABLE 2-16: The Effect of Explicitly Representing Methyl Nitrite

HC/NOx Ratio	Control Mixture	Reduction or Substitution	Date	Formaldehyde is produced earlier.	More formaldehyde is produced.
3:1	SynAuto	1/3 MEOH w/ 0% HCHO	Au0784	Yes	No
9:1	SynAuto	1/3 MEOH w/20% HCHO	Au0884	Yes	No
3:1	SynAuto	1/3 MEOH w/20% HCHO	Au0984	Yes	No
9:1	SynUrban	1/3 MEOH w/20% HCHO	Au2284	Yes	Yes

TABLE 2-17: The Effects of Different Wall Models

HC/NOx	Control	Reduction or	Date	Wall Model with Best Agreement		
Ratio	Mixture	Substitution		Ozone	HCHO	PAN
9:1	SynUrban	1/3 MEOH w/ 0% HCHO	St0184	None	None	None
3:1	SynAuto	1/3 MEOH w/10% HCHO	Au0484	Killus	None	Killus
3:1	SynUrban	1/3 MEOH w/10% HCHO	Au2584	None	Killus	None
9:1	SynAutoUrban	1/3 MEOH w/ 0% HCHO	St1784	None	Killus	None

Analysis of the HCHO Chemistry

I explained earlier that there is concern that large-scale use of MFVs may increase ambient concentrations of formaldehyde. Even though a smog chamber is not a good surrogate for the ambient atmosphere, it is interesting to look at the differences in maximum concentrations of formaldehyde between the control side and reduction/ substitution side of the chamber. See Table 2-18. There is no clear pattern of increasing formaldehyde concentrations in the chamber due to methanol substitution. The only experiments that do show a significant increase in formaldehyde due to methanol substitution are those with the least reactive pollutant mixture, SynUrban at an HC/NO_x ratio of 3/1. Furthermore, methanol substitution did not effect the ability of the chemical mechanisms to predict formaldehyde concentrations. This suggests that there is some large source of formaldehyde which is dependent on the control mixture of hydrocarbons and is not significantly affected by methanol substitution.

To investigate this possibility, I applied an integrated rate/mass balance (IR/MB) analysis technique developed by Jeffries [1984] to the mechanism predictions for several of the chamber experiments. For use in this analytical technique, PC-PKSS integrates the reaction rates between each time step by assuming that the change in concentrations between time steps is linear. The integrated

TABLE 2-18: The Change in Formaldehyde Maxima Due to Reduction or Substitution

HC/NOx Ratio	Control Mixture	Reduction or Substitution	Date	Ratio of Red/Substitution Side HCHO Max to Control Side HCHO Max	
9:1	SynAuto	1/3 HC reduction	Au0684	1.00	same
		1/3 MEOH w/20% HCHO	Au0884	0.98	same
	SynUrban	1/3 HC reduction	Jn2685	0.69	inc
		1/3 MEOH w/ 0% HCHO	St0184	0.90	same
		1/3 MEOH w/20% HCHO	Au2284	1.03	same
3:1	SynAuto	1/3 HC reduction	Au0584	0.76	dec
		1/3 MEOH w/ 0% HCHO	Au0784	0.88	dec
		1/3 MEOH w/10% HCHO	Au0484	1.00	same
		1/3 MEOH w/20% HCHO	Au0984	1.07	same
	SynUrban	1/3 HC reduction	St0284	1.12	inc
		1/3 MEOH w/10% HCHO	Au2584	1.14	inc
		1/3 MEOH w/10% HCHO	Jn2885	1.56	inc
		1/3 MEOH w/20% HCHO	St0384	1.50	inc
9:1	SynAutoUrban	1/3 HC reduction	St0884	?	?
		1/3 MEOH w/10% HCHO	St1784	0.86	dec
		HCHO addition	St2184	1.21	inc
	HMWMIX	1/3 HC reduction	St1984	0.54	dec

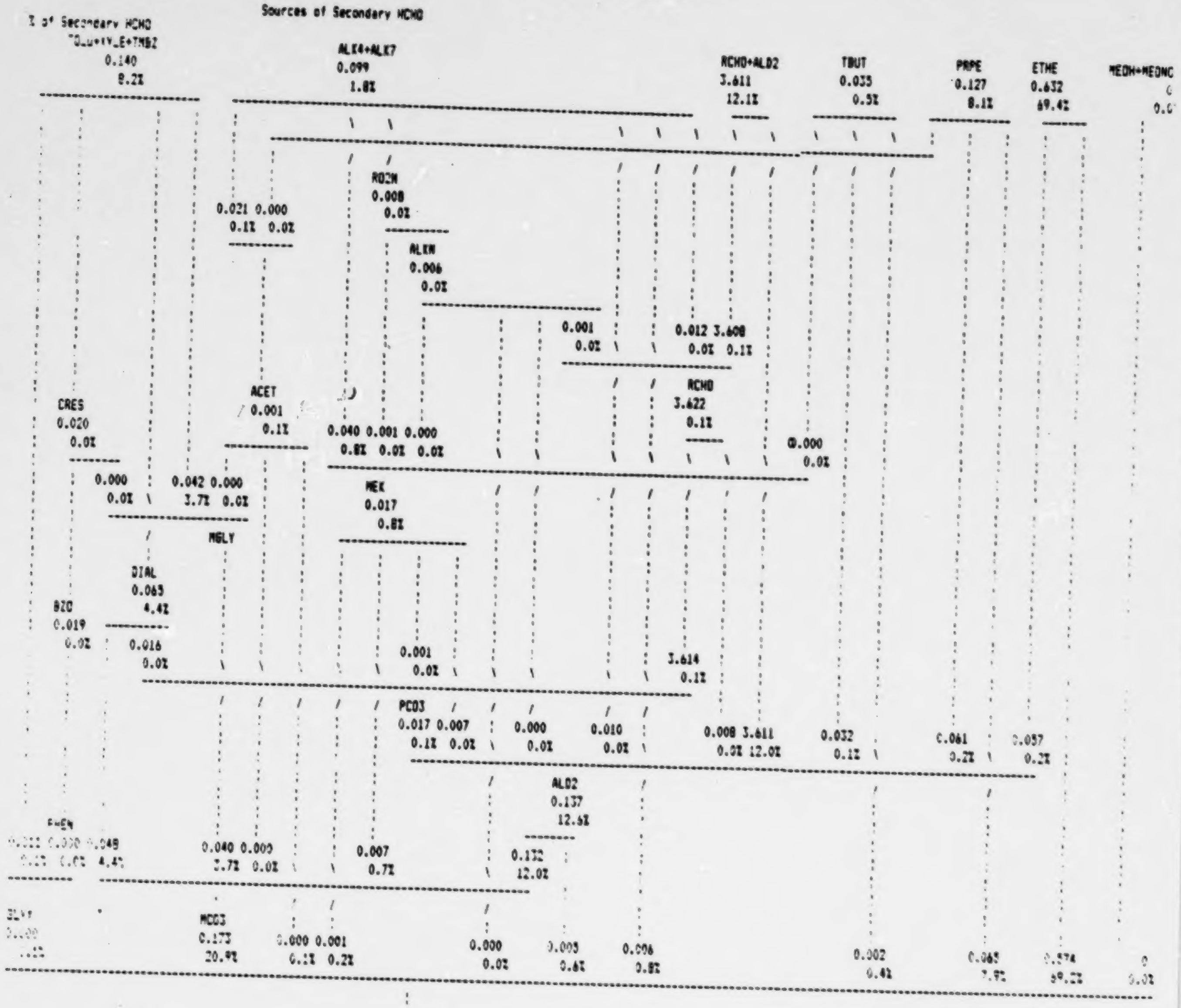
rates for each reaction are summed over the entire simulation. By multiplying by the stoichiometric coefficient of a species in a given reaction, the integrated reaction rate becomes the mass of the species produced or consumed by that reaction pathway during the simulation. By including these masses in a flowchart of the production and consumption pathways of formaldehyde, I calculated the contribution of each emitted species to the total formaldehyde produced during a simulation.

Two experiments, Au0884 and Jn2885, were selected for this analysis based on the representativeness of the mixtures used and the quality of the model predictions. Formaldehyde mass balance flowcharts were constructed for CAL and CB4 and applied to each side of the chamber for each experiment. These flowcharts are shown in Figures 2-8 through 2-15. The non-formaldehyde hydrocarbon species are listed in groups across the top of each chart. Listed under each species or group of species is the total mass and percentage of secondary formaldehyde that was produced from initial concentrations of that hydrocarbon species. Descending from the top of the chart are the pathways by which secondary formaldehyde is produced. Near the bottom of the chart the pathways converge and the total mass of secondary formaldehyde is listed. This mass is compared to the amount of initial formaldehyde and the total formaldehyde generated throughout the simulation. Below the final concentration of formaldehyde, the pathways of formaldehyde consumption are listed.

Figure 2-8: Pathway Analysis for Au0884, Blue, CAL

```
PATHWAY ANALYSIS OF HCHO CHEMISTRY FOR CAL.

Run description:  August 8, 1984 3.7 ppmC SYNAUTO (BLUE)
                  Carter, Atkinson, Lurman, Chamber Version 3.2, w/Carter's wall model at 11/16/88 22:45:53
                  T=600.0
```



Sources of Secondary HCHO
% of Secondary HCHO
TOLU+XYLE+TMBZ 0.140 8.2%
ALK4+ALK7 0.099 1.8%
RCHO+ALD2 3.611 12.1%
TBUT 0.035 0.5%
PRPE 0.127 8.1%
ETHE 0.632 69.4%
MEOH+MEONO
RO2N 0.008 0.0%
0.021 0.000 0.1% 0.0%
ALKN 0.006 0.0%
0.001 0.0%
0.012 3.608 0.0% 0.1%
RCHO 3.622 0.1%
CRES 0.020 0.0%
ACET 0.001 0.1%
0.040 0.001 0.000 0.8% 0.0% 0.0%
0.000 0.0%
0.000 0.0%
0.042 0.000 3.7% 0.0%
MEK 0.017 0.8%
MGLY
DIAL 0.063 4.4%
BZO 0.019 0.0%
0.016 0.0%
0.001 0.0%
3.614 0.1%
PCO3 0.017 0.007 0.1% 0.0%
0.000 0.0%
0.010 0.0%
0.008 3.611 0.0% 12.0%
0.032 0.1%
0.061 0.2%
0.057 0.2%
ALD2 0.137 12.6%
PHEN
0.048 4.4%
0.040 0.000 3.7% 0.0%
0.007 0.7%
0.132 12.0%
GLY
MCO3 0.173 20.9%
0.000 0.001 0.1% 0.2%
0.000 0.0%
0.005 0.6%
0.006 0.8%
0.002 0.4%
0.065 7.9%
0.574 59.2%
0.0%

```
% of Total HCHO   Initial   0.057        Secondary   0.830                        0.003 Background
                  HCHO       6.4%        HCHO         93.2%                        0.4%HCHO
                           -----------------------------------------------------------------
                                         Total HCHO  0.891
                                         Final conc. 0.243

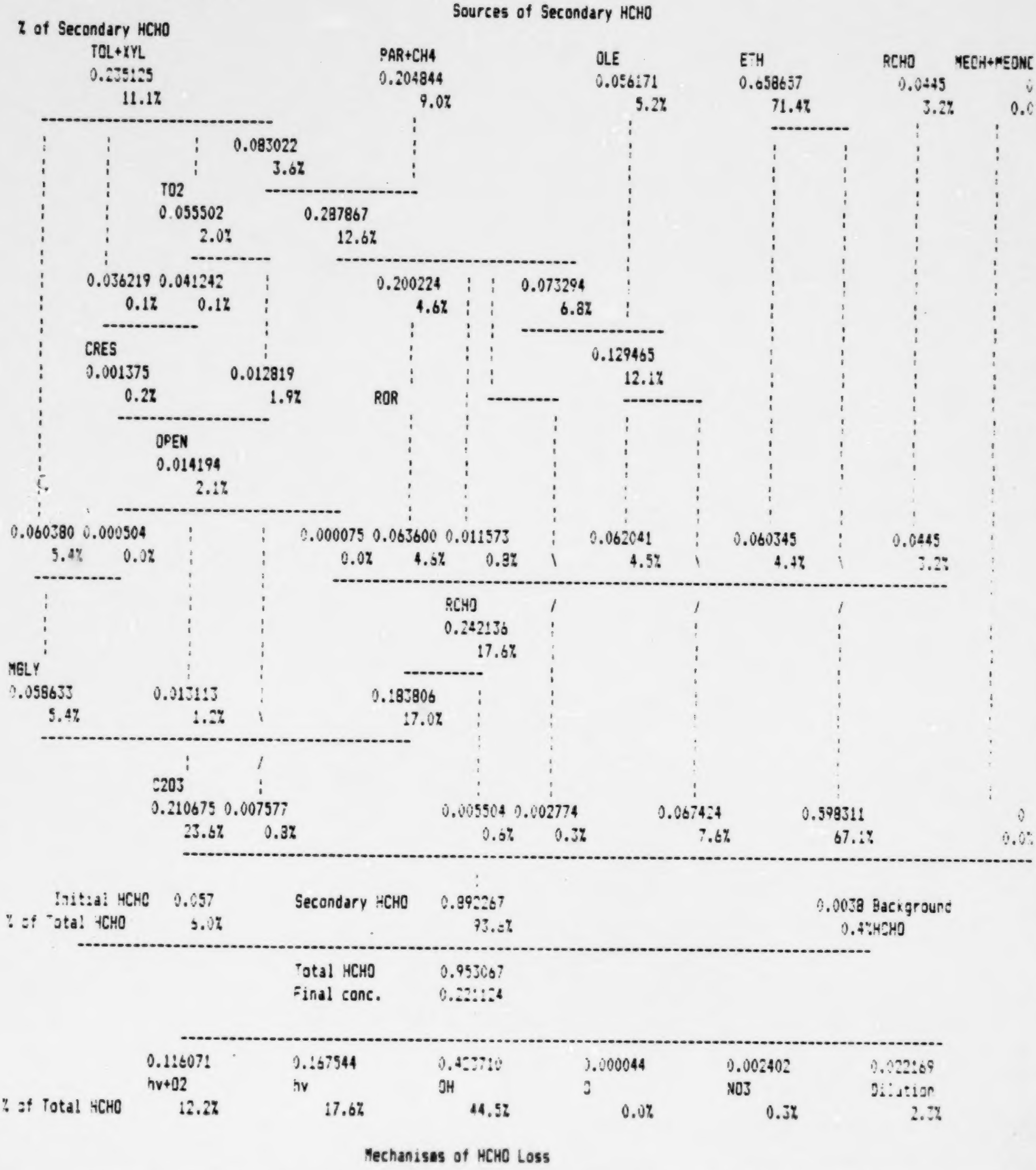
                                 ---------------------------------------------------------------
                                 0.113      0.164      0.322      0.003      0.019      0.024
% of Total HCHO                  hv+O2      hv         OH         NO3        HO2        Dilution
                                  12.8%     18.3%      36.2%       0.4%       2.1%       2.7%

                                            Mechanisms of HCHO Loss
```

Figure 2-9: Pathway Analysis for Au0884, Blue, CB4

```
PATHWAY ANALYSIS OF HCHO CHEMISTRY FOR CB4.2

Run description:  August 8, 1984 3.7 ppmC SYNAUTO (BLUE)
                  Carbon Bond Four.Two, Chamber Version Sub3.2, w/Carter's wall model at 11/16/88 22:49:14
                  T=600.0
```

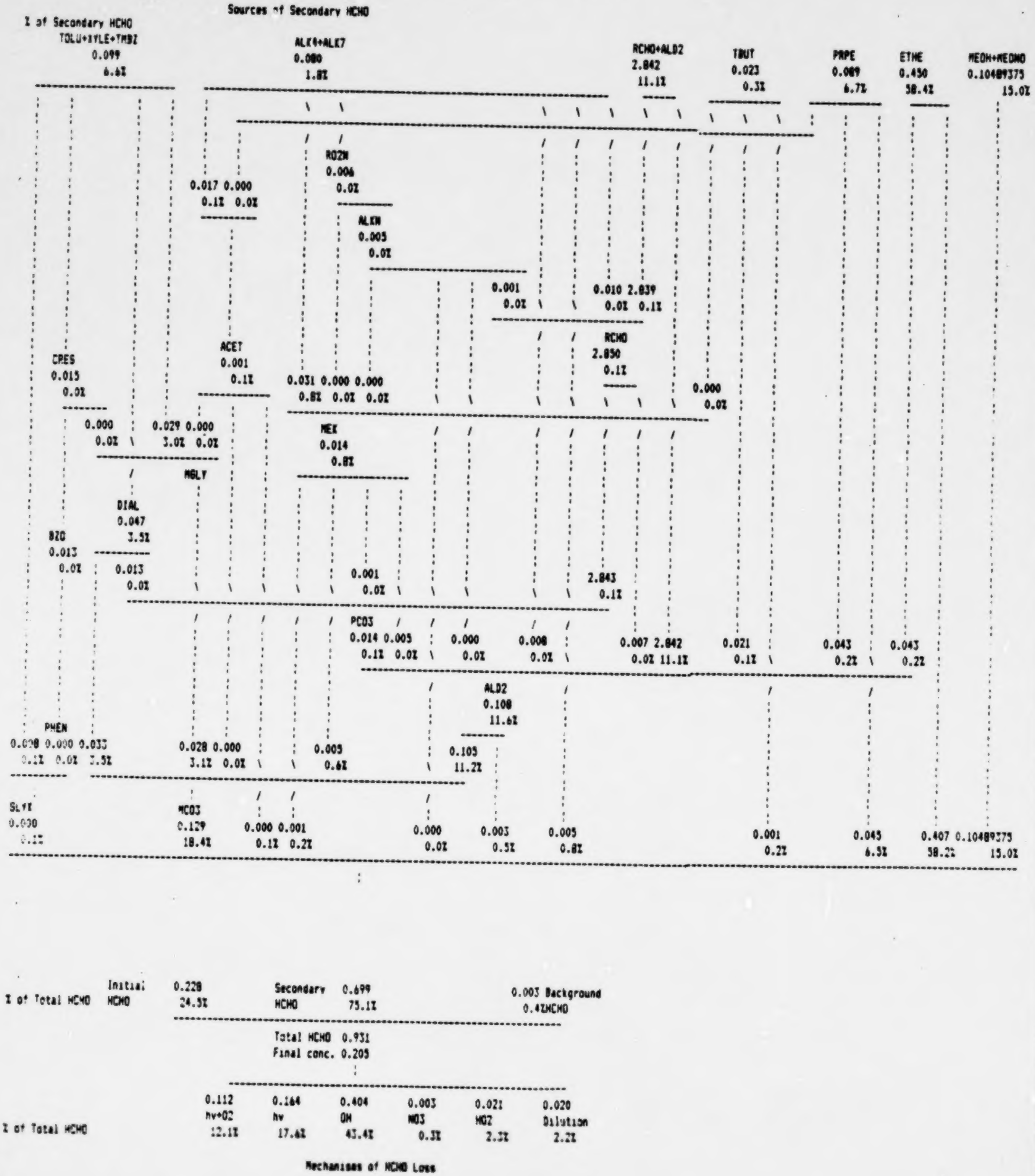


Sources of Secondary HCHO
% of Secondary HCHO
TOL+XYL 0.235125 11.1%
PAR+CH4 0.204844 9.0%
OLE 0.056171 5.2%
ETH 0.658657 71.4%
RCHO 0.0445 3.2%
MEOH+MEONC 0 0.0
0.083022 3.6%
TO2 0.055502 2.0%
0.287867 12.6%
0.036219 0.1%
0.041242 0.1%
0.200224 4.6%
0.073294 6.8%
CRES 0.001375 0.2%
0.012819 1.9%
0.129465 12.1%
ROR
OPEN 0.014194 2.1%
0.060380 5.4%
0.000504 0.0%
0.000075 0.0%
0.063600 4.6%
0.011573 0.8%
0.062041 4.5%
0.060345 4.4%
0.0445 3.2%
RCHO 0.242136 17.6%
MGLY 0.058633 5.4%
0.013113 1.2%
0.183806 17.0%
C2O3 0.210675 23.6%
0.007577 0.8%
0.005504 0.6%
0.002774 0.3%
0.067424 7.6%
0.598311 67.1%
0 0.0%
Initial HCHO 0.057
% of Total HCHO 6.0%
Secondary HCHO 0.892267 93.6%
0.0038 Background 0.4%HCHO
Total HCHO 0.953067
Final conc. 0.221124
0.116071 hv+O2 12.2%
0.167544 hv 17.6%
0.423710 OH 44.5%
0.000044 O 0.0%
0.002402 NO3 0.3%
0.022169 Dilution 2.3%
% of Total HCHO
Mechanisms of HCHO Loss

Figure 2-10: Pathway Analysis for Au0884, Red, CAL

PATHWAY ANALYSIS OF HCHO CHEMISTRY FOR CAL.

Run description: August 8, 1984 2.5 ppmC SYNAUTO, 0.79 ppm MeOH, 0.23 ppm HCHO (RED)
Carter, Atkinson, Lurman, Chamber Version 3.2, w/Carter's wall model at 04/26/89 19:37:48
T=600.0



Sources of Secondary HCHO
% of Secondary HCHO
TOLU+XYLE+TMBZ 0.099 6.6%
ALK4+ALK7 0.080 1.8%
RCHO+ALD2 2.842 11.1%
TBUT 0.023 0.3%
PRPE 0.089 6.7%
ETHE 0.450 58.4%
MEOH+MEOHO 0.10489375 15.0%
0.017 0.000 0.1% 0.0%
RO2N 0.006 0.0%
ALKN 0.005 0.0%
0.001 0.0%
0.010 2.839 0.0% 0.1%
RCHO 2.850 0.1%
CRES 0.015 0.0%
ACET 0.001 0.1%
0.031 0.000 0.000 0.8% 0.0% 0.0%
0.000 0.0%
0.000 0.0%
0.029 0.000 3.0% 0.0%
MEK 0.014 0.8%
MGLY
DIAL 0.047 3.5%
BZO 0.013 0.0%
0.013 0.0%
0.001 0.0%
2.843 0.1%
PCO3
0.014 0.005 0.1% 0.0%
0.000 0.0%
0.008 0.0%
0.007 2.842 0.0% 11.1%
0.021 0.1%
0.043 0.2%
0.043 0.2%
ALD2 0.108 11.6%
PHEN
0.028 0.000 0.033 0.1% 0.0% 3.5%
0.028 0.000 3.1% 0.0%
0.005 0.6%
0.105 11.2%
SLYI 0.030 0.1%
MCO3 0.129 18.4%
0.000 0.001 0.1% 0.2%
0.000 0.0%
0.003 0.5%
0.005 0.8%
0.001 0.2%
0.045 6.5%
0.407 58.2%
0.10489375 15.0%
% of Total HCHO
Initial HCHO 0.228 24.5%
Secondary HCHO 0.699 75.1%
0.003 Background 0.4%HCHO
Total HCHO 0.931
Final conc. 0.205
0.112 hv+O2 12.1%
0.164 hv 17.6%
0.404 OH 43.4%
0.003 NO3 0.3%
0.021 HO2 2.3%
0.020 Dilution 2.2%
% of Total HCHO
Mechanisms of HCHO Loss

Figure 2-11: Pathway Analysis for Au0884, Red, CB4

PATHWAY ANALYSIS OF HCHO CHEMISTRY FOR CB4.2

Run description: August 8, 1984 2.5 ppmC SYNAUTO, 0.79 ppm MeOH, 0.23 ppm HCHO (RED)
Carbon Bond Four.Two, Chamber Version Sub3.2, w/Carter's wall model at 04/26/89 19:36:12
T=600.0

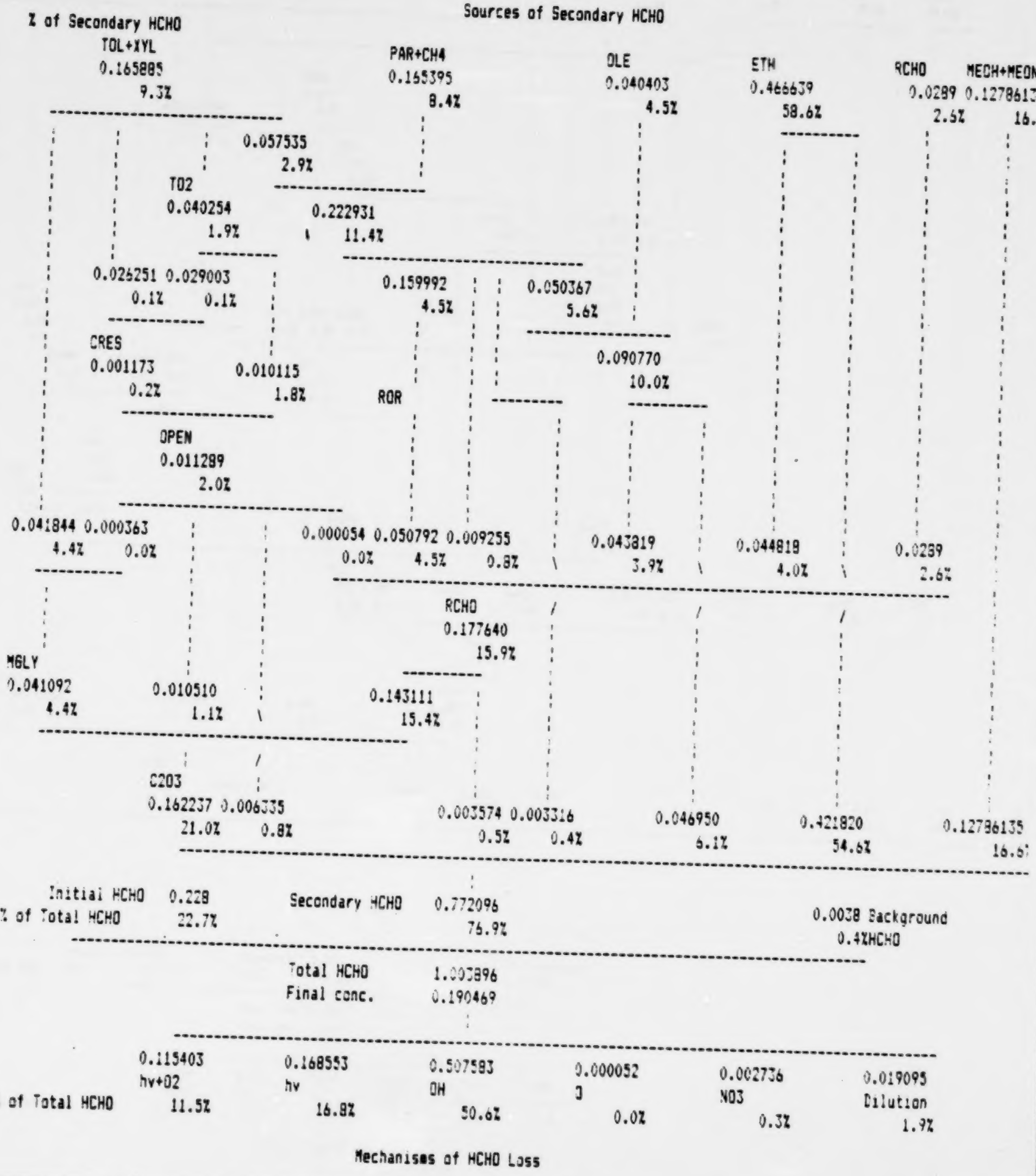

Sources of Secondary HCHO
% of Secondary HCHO
TOL+XYL 0.165885 9.3%
PAR+CH4 0.165395 8.4%
OLE 0.040403 4.5%
ETH 0.466639 58.6%
RCHO 0.0289 2.6%
MEOH+MEONO 0.12786135 16.6
0.057535 2.9%
TO2 0.040254 1.9%
0.222931 11.4%
0.026251 0.1%
0.029003 0.1%
0.159992 4.5%
0.050367 5.6%
CRES 0.001173 0.2%
0.010115 1.8%
ROR
0.090770 10.0%
OPEN 0.011289 2.0%
0.041844 4.4%
0.000363 0.0%
0.000054 0.0%
0.050792 4.5%
0.009255 0.8%
0.043819 3.9%
0.044819 4.0%
0.0289 2.6%
RCHO 0.177640 15.9%
MGLY 0.041092 4.4%
0.010510 1.1%
0.143111 15.4%
C2O3 0.162237 21.0%
0.006335 0.8%
0.003574 0.5%
0.003316 0.4%
0.046950 6.1%
0.421820 54.6%
0.12786135 16.6%
Initial HCHO 0.228
% of Total HCHO 22.7%
Secondary HCHO 0.772096 76.9%
0.0038 Background 0.4%HCHO
Total HCHO 1.003896
Final conc. 0.190469
0.115403 hv+O2 11.5%
0.168553 hv 16.8%
0.507583 OH 50.6%
0.000052 O 0.0%
0.002736 NO3 0.3%
0.019095 Dilution 1.9%
% of Total HCHO
Mechanisms of HCHO Loss

Figure 2-12: Pathway Analysis for Jn2885, Red. CAL

PATHWAY ANALYSIS OF HCHO CHEMISTRY FOR CAL.

Run description: JUNE 28, 1985 1.24 ppmC SYNURBAN (RED)
Carter, Atkinson, Lurman, Chamber Version 3.2, w/Carter's wall model at 11/16/88 23:19:07
T=600.0

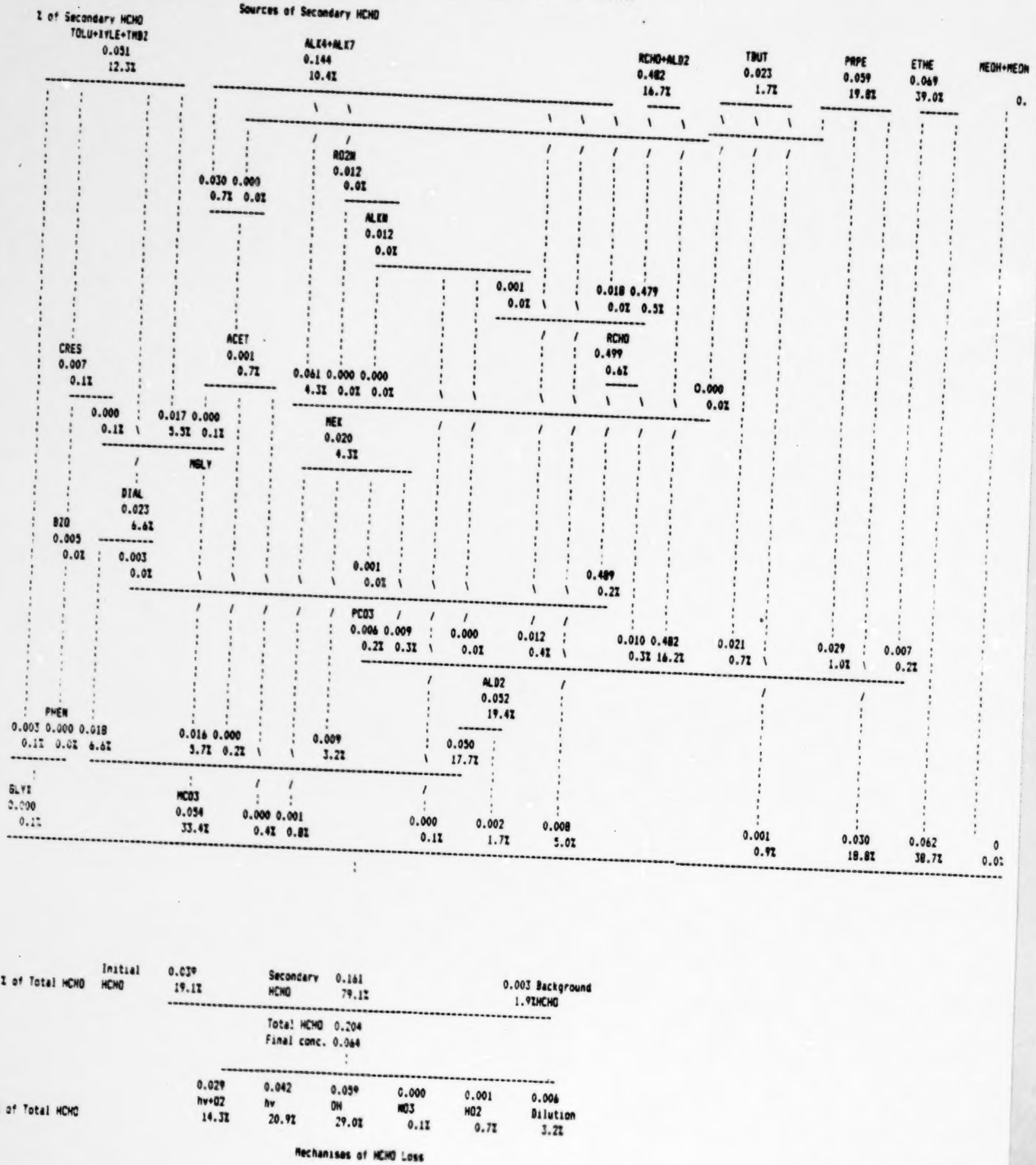

% of Secondary HCHO
Sources of Secondary HCHO
TOLU+XYLE+TMB2 0.031 12.3%
ALK4+ALK7 0.144 10.4%
RCHO+ALD2 0.482 16.7%
TBUT 0.023 1.7%
PRPE 0.059 19.8%
ETHE 0.069 39.0%
MEOH+MEOH 0.
RO2N 0.012 0.0%
0.030 0.000 0.7% 0.0%
ALKN 0.012 0.0%
0.001 0.0%
0.018 0.479 0.0% 0.5%
RCHO 0.499 0.6%
CRES 0.007 0.1%
ACET 0.001 0.7%
0.061 0.000 0.000 4.3% 0.0% 0.0%
0.000 0.0%
0.000 0.1%
0.017 0.000 5.3% 0.1%
MEK 0.020 4.3%
MGLY
DIAL 0.023 6.6%
BZO 0.005 0.0%
0.003 0.0%
0.001 0.0%
0.489 0.2%
PCO3 0.006 0.009 0.2% 0.3%
0.000 0.0%
0.012 0.4%
0.010 0.482 0.3% 16.2%
0.021 0.7%
0.029 1.0%
0.007 0.2%
ALD2 0.052 19.4%
PHEN 0.003 0.000 0.018 0.1% 0.0% 6.6%
0.016 0.000 3.7% 0.2%
0.009 3.2%
0.050 17.7%
GLYX 0.000 0.1%
HCO3 0.054 33.4%
0.000 0.001 0.4% 0.8%
0.000 0.1%
0.002 1.7%
0.008 5.0%
0.001 0.9%
0.030 18.8%
0.062 38.7%
0 0.0%
% of Total HCHO
Initial HCHO 0.039 19.1%
Secondary HCHO 0.161 79.1%
0.003 Background 1.9%HCHO
Total HCHO 0.204
Final conc. 0.064
% of Total HCHO
0.029 hv+O2 14.3%
0.042 hv 20.9%
0.059 OH 29.0%
0.000 NO3 0.1%
0.001 HO2 0.7%
0.006 Dilution 3.2%
Mechanisms of HCHO Loss

Figure 2-13: Pathway Analysis for Jn2885, Red, CB4

```
   PATHWAY ANALYSIS OF HCHO CHEMISTRY FOR CB4.2

   Run description:  JUNE 28, 1985 2.39 ppmC SYNURBAN (RED)
                     Carbon Bond Four.Two, Chamber Version Sub3.2, w/Carter's wall model at 11/16/88 23:21:28
                     T=600.0

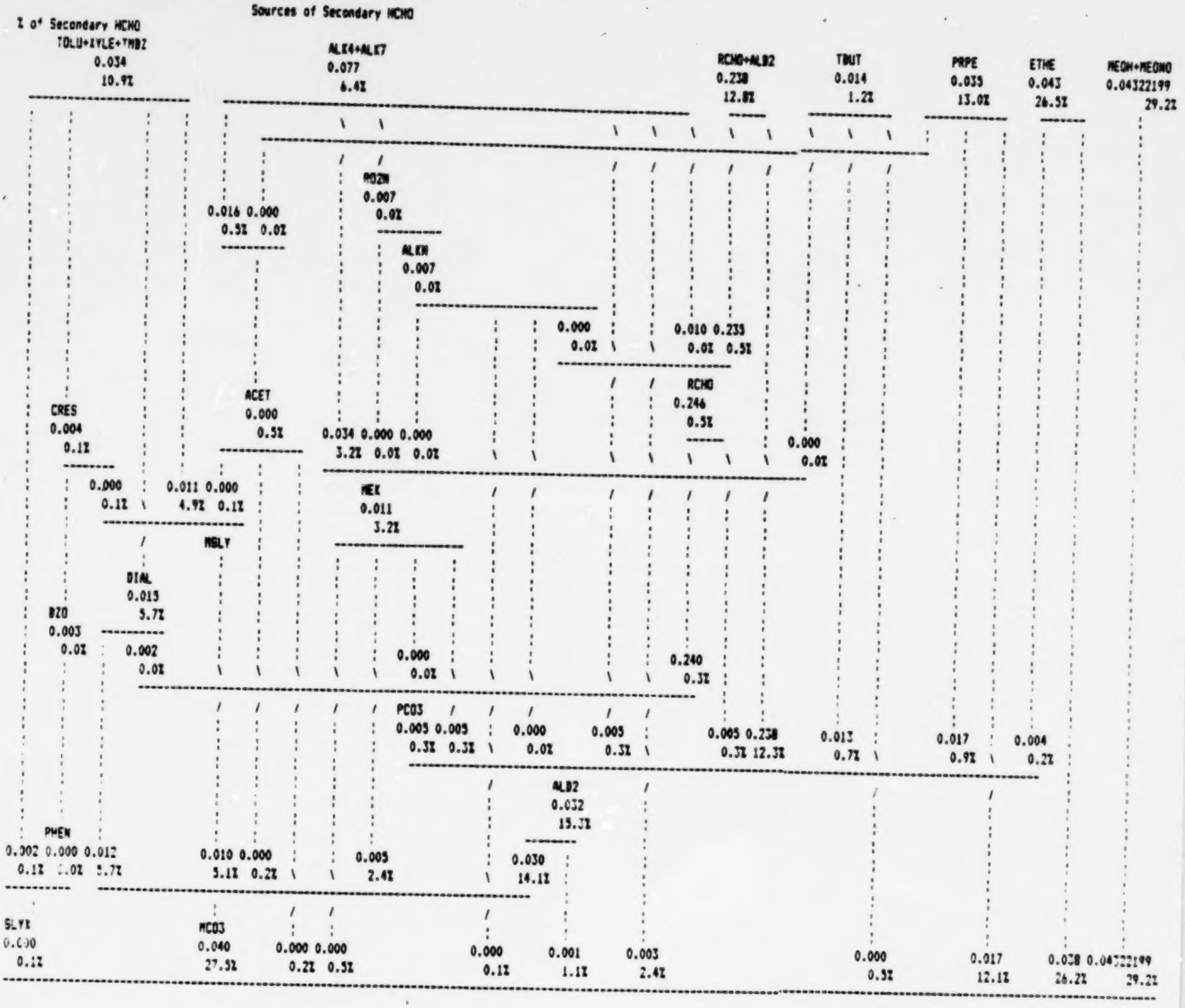
                                                        Sources of Secondary HCHO
   % of Secondary HCHO
            TOL+XYL                        PAR+CH4                    OLE               ETH               RCHO   MEOH+MEONO
           0.076470                        0.173595                   0.027482          0.062640           0.0213        0
               19.3%                           25.4%                      12.4%             37.6%              5.3%    0.0
     ------------------------------                :                                    ----------
     :       :          :    0.029272              :                         :                 :        :       :         :
     :       :          :          4.3%            :                         :                 :        :       :         :
     :       :      TO2          --------------------                        :                 :        :       :         :
     :       :      0.015655          0.202868                               :                 :        :       :         :
     :       :           6.0%             29.7%                              :                 :        :       :         :
     :       :           ----------       ------------------------------     :                 :        :       :         :
     :     0.010254 0.005878     :            0.158848   :  :  0.032657      :                 :        :       :         :
     :         0.4%     0.2%     :                11.7%  :  :      14.7%     :                 :        :       :         :
     :       ------------        :                  :    :  :  ------------------              :        :       :         :
     :     CRES                  :                  :    :  :                                  :        :       :         :
     :                           :                  :    :  :        0.060140                  :        :       :         :
     :     0.000982        0.008797                 :    :  :            27.1%                 :        :       :         :
     :         0.6%            5.8%           ROR        :  ---------    ----------            :        :       :         :
     :        --------------------              :    :          :        :        :            :        :       :         :
     :             OPEN                         :    :          :        :        :            :        :       :         :
     :             0.009780                     :    :          :        :        :            :        :       :         :
     :                 6.4%                     :    :          :        :        :            :        :       :         :
     :        -----------------------------     :    :          :        :        :            :        :       :         :
 0.021288 0.000202      :        :    0.000030 0.046811 0.010179   :    0.029263   :     0.006415     :     0.0213      :
      3.6%     0.1%     :        :         0.0%   11.7%     2.5%   \         7.3%  \         1.6%     \        5.3%     :
    -----------         :        :        ---------------------------------------------------------------------------   :
     :                  :        :                   RCHO          /                 /                  /               :
     :                  :        :                   0.114001      :                 :                  :               :
     :                  :        :                       28.4%     :                 :                  :               :
 MGLY                   :        :               ----------        :                 :                  :               :
 0.019104          0.009051      :            0.057430   :         :                 :                  :               :
      8.7%             4.1%      \                26.1%  :         :                 :                  :               :
    ----------------------------------------------       :         :                 :                  :               :
     .                  :        /                       :         :                 :                  :               :
                 C2O3            :                       :         :                 :                  :               :
                 0.060824 0.003483                   0.003520 0.001182          0.030876          0.056224               0
                     39.0%     2.2%                      2.3%     0.8%              19.9%             36.0%            0.0
                     --------------------------------------------------------------------------------------------------------
                                                         :
      Initial HCHO    0.039         Secondary HCHO    0.156112
 % of Total HCHO       19.6%                              78.5%                                        0.0038 Background
                                                                                                           1.9%HCHO
         --------------------------------------------------------------------------------------------------
                                    Total HCHO        0.198912
                                    Final conc.       0.068494
                                                         :
                     ----------------------------------------------------------------------------------------------
                 0.029110          0.042482          0.051900          0.000018          0.000139          0.006867
                 hv+O2             hv                OH                O                 NO3               Dilution
 % of Total HCHO     14.6%             21.4%             26.0%              0.0%              0.1%              3.5%

                                            Mechanisms of HCHO Loss
```

Figure 2-14: Pathway Analysis for Jn2885, Blue, CAL

```
PATHWAY ANALYSIS OF HCHO CHEMISTRY FOR CAL.

Run description:  June 28, 1985 1.32 ppmC SYNURBAN, 0.38 ppm MeOH, 0.7 ppm HCHO (BLUE)
                  Carter, Atkinson, Lurman, Chamber Version 3.2, w/Carter's wall model at 11/16/88 23:16:08
                  T=600.0
```


Sources of Secondary HCHO
% of Secondary HCHO
TOLU+XYLE+TMBZ 0.034 10.9%
ALK4+ALK7 0.077 6.4%
RCHO+ALD2 0.238 12.8%
TBUT 0.014 1.2%
PRPE 0.035 13.0%
ETHE 0.043 26.5%
MEOH+MEONO 0.04322199 29.2%
0.016 0.000 0.5% 0.0%
RO2N 0.007 0.0%
ALKN 0.007 0.0%
0.000 0.0%
0.010 0.235 0.0% 0.5%
ACET 0.000 0.5%
RCHO 0.246 0.5%
CRES 0.004 0.1%
0.034 0.000 0.000 3.2% 0.0% 0.0%
0.000 0.0%
0.000 0.1%
0.011 0.000 4.9% 0.1%
MEK 0.011 3.2%
MGLY
DIAL 0.013 5.7%
BZO 0.003 0.0%
0.002 0.0%
0.000 0.0%
0.240 0.3%
PCO3 0.005 0.005 0.3% 0.3%
0.000 0.0%
0.005 0.3%
0.005 0.238 0.3% 12.3%
0.013 0.7%
0.017 0.9%
0.004 0.2%
ALD2 0.032 15.3%
PHEN
0.002 0.000 0.012 0.1% 0.0% 5.7%
0.010 0.000 5.1% 0.2%
0.005 2.4%
0.030 14.1%
SLYX 0.000 0.1%
MCO3 0.040 27.5%
0.000 0.000 0.2% 0.5%
0.000 0.1%
0.001 1.1%
0.003 2.4%
0.000 0.5%
0.017 12.1%
0.038 26.2%
0.04322199 29.2%

```
                 Initial    0.090        Secondary  0.148                 0.003 Background
% of Total HCHO  HCHO        37.4%       HCHO        61.0%                  1.6%HCHO
                            --------------------------------------------------------------
                                         Total HCHO  0.242
                                         Final conc. 0.070
                                                       :
                                   -----------------------------------------------------
                                0.036     0.053     0.074     0.000     0.001     0.007
                                hv+O2     hv        OH        NO3       HO2       Dilution
% of Total HCHO                  14.9%     21.9%     30.8%      0.1%      0.5%      2.9%

                                               Mechanisms of HCHO Loss
```

Figure 2-15: Pathway Analysis for Jn2885, Blue, CB4

```
PATHWAY ANALYSIS OF HCHO CHEMISTRY FOR CB4.2

Run description:  June 28, 1985 1.32 ppmC SYNURBAN, 0.58 ppm MeOH, 0.07 ppm HCHO (BLUE)
                  Carbon Bond Four.Two, Chamber Version Sub3.2, w/Carter's wall model at 11/16/88 23:18:12
                  T=600.0

                                          Sources of Secondary HCHO
% of Secondary HCHO
        TOL+XYL                    PAR+CH4             OLE           ETH           RCHO    MEOH+MEONO
       0.052289                   0.091741             0.016784      0.040254        0.0125 0.04033992
          16.7%                      16.7%                 8.5%         26.2%          4.0%     27.9
   ----------------------                 :                   :         --------       :        :
   :     :       :   0.019951             :                   :         :      :       :        :
   :     :       :       3.6%             :                   :         :      :       :        :
   :     :    TO2        ----------------                     :         :      :       :        :
   :     :    0.010772     0.111692                           :         :      :       :        :
   :     :       5.4%         20.3%                           :         :      :       :        :
   :     :       --------     ------------------------        :         :      :       :        :
   :  0.007054 0.003312 :       0.085987  :  :  0.018914      :         :      :       :        :
   :      0.5%    0.2%  :           8.1%  :  :      9.6%      :         :      :       :        :
   :    --------        :           :     :  :  ------------------      :      :       :        :
   :  CRES              :           :     :  :        0.035698          :      :       :        :
   :  0.000905       0.006713       :     :  :           18.2%          :      :       :        :
   :      0.7%           5.2%   ROR       :  --------    --------       :      :       :        :
   :    ---------------         :     :       :        :      :         :      :       :        :
   :          OPEN              :     :       :        :      :         :      :       :        :
   :          0.007618          :     :       :        :      :         :      :       :        :
   :              5.9%          :     :       :        :      :         :      :       :        :
   :    -------------------     :     :       :        :      :         :      :       :        :
0.014510 0.000120   :     :  0.000018 0.025257 0.005533 :   0.017518 :  0.004355  :    0.0125   :
   7.2%      0.1%   :     :      0.0%   8.1%   1.8%     \       5.6% \       1.4% \       4.0%  :
  ----------        :     :    -----------------------------------------------------------     :
   :                :     :             RCHO        /              /             /              :
   :                :     :             0.065182    :              :             :              :
   :                :     :                20.3%    :              :             :              :
MGLY                :     :             --------    :              :             :              :
0.013192         0.007074 :          0.035167  :    :              :             :              :
   7.3%              3.9% \             19.4%  :    :              :             :              :
   ----------------------------------------    :    :              :             :              :
                    :     /                    :    :              :             :              :
             C2O3         :                    :    :              :             :              :
             0.044175 0.002777          0.002035 0.001257     0.018179      0.035899     0.04033992
                30.5%     1.9%               1.4%    0.9%        12.6%         24.3%          27.9
                ---------------------------------------------------------------------------------

     Initial HCHO  0.0908        Secondary HCHO   0.144665                        0.0038 Background
% of Total HCHO    37.9%                             60.5%                          1.6%HCHO
       -------------------------------------------------------------------------------------

                             Total HCHO       0.239265
                             Final conc.      0.072743

                ------------------------------------------------------------------------
                 0.036192         0.053409        0.069967      0.000022      0.000077      0.007252
                 hv+O2            hv              OH            O             NO3           Dilution
% of Total HCHO    15.1%             22.3%           29.2%          0.0%          0.0%          3.0%

                                       Mechanisms of HCHO Loss
```

The final concentrations listed in the flowcharts differ from the actual predictions of the mechanisms because of errors introduced by the integration method and by the estimation of the effect of dilution. While the rate of dilution is relatively constant throughout the chamber experiments, the mass of formaldehyde lost is proportional to its concentration. Because the concentration of formaldehyde is changing throughout the experiment, the total loss of formaldehyde due to dilution must be estimated by the integrated rate of dilution multiplied by the difference between the total mass of formaldehyde produced and the sum of all other loss pathways.

Secondary production of formaldehyde accounts for approxiamately 93% of the total formaldehyde produced for SynAuto and approxiamately 79% for SynUrban. With 33% methanol substitution, the contribution of secondary production drops 20% to an average of 76% and 61% for SynAuto and SynUrban, respectively. Table 2-19 summarizes the contribution of groups of hydrocarbon species to the initial mix of hydrocarbons as compared their contribution to the production of secondary formaldehyde. It is difficult to compare the contributions of alkanes because of the very different ways they are represented in the two mechanisms. The contribution of species which are represented explicitly in both mechanisms, such as methanol or ethylene, are easier to compare. The contribution of methanol to secondary formaldehyde is approxiamately

The final concentrations listed in the flowcharts differ from the actual predictions of the mechanisms because of errors introduced by the integration method and by the estimation of the effect of dilution. While the rate of dilution is relatively constant throughout the chamber experiments, the mass of formaldehyde lost is proportional to its concentration. Because the concentration of formaldehyde is changing throughout the experiment, the total loss of formaldehyde due to dilution must be estimated by the integrated rate of dilution multiplied by the difference between the total mass of formaldehyde produced and the sum of all other loss pathways.

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TABLE 2-19: Percentage of Non-Formaldehyde Hydrocarbon Emissions (E%) vs. Percentage of Secondary Formaldehyde Formation (S%)

Date	Au0884				Jn2885			
HC/NOx Ratio	9:1				3:1			
Hydrocarbon Mixture	SynAuto		1/3 MEOH w/20% HCHO		SynUrban		1/3 MEOH w/10% HCHO	
Hydrocarbon Class	E%	S%	E%	S%	E%	S%	E%	S%
CB4								
PAR+CH4	25.4	9.0	19.0	8.4	65.4	25.4	41.2	16.7
ETH	29.5	71.4	22..2	58.6	6.2	37.6	4.9	26.2
OLE+RCHO	7.0	8.4	5.1	7.1	5.2	17.7	3.9	12.5
TOL+XYL	38.1	11.1	29.0	9.3	23.2	19.3	19.0	19.3
MEOH	0	0	24.8	16.6	0	0	31.0	27.9
CAL								
ALK4+ALK7	23.3	1.8	16.2	1.8	65.5	10.4	42.9	6.4
ETHE	29.2	69.4	22.4	58.4	5.8	39.0	4.6	26.5
PRPE+TBUT+RCHO+ALD2	9.1	20.7	6.8	18.1	6.8	38.2	5.1	27.0
TOLU+XYLE+TMBZ	38.4	8.2	29.7	6.6	21.9	12.3	18.2	10.9
MEOH	0	0	25.0	15.0	0	0	29.2	29.2

Chamber Mixtures vs. Ambient Air

The comparison of the model predictions and chamber observations showed that the performance of the chemical mechanisms is dependent on the existing composition of ambient hydrocarbons. The analysis of the formaldehyde chemistry revealed that the impact of MFVs on ambient formaldehyde levels also is dependent on the existing composition of ambient hydrocarbons. Past research summarized in Part 1 concluded that the impacts of MFVs on ozone show this same dependence. The relevancy of the evaluation and analysis in this report is dependent, therefore, on how representative of present and future urban mixtures are the mixtures used in the chamber experiments.

Jeffries et al. [1988b] analyzed the results from an on-going effort by EPA to gather speciated hydrocarbon measurements from urban atmospheres. Using the average of 66 city-years of speciated hydrocarbon measurements and recommendations from model developers, Jeffries et al. developed a recommended default hydrocarbon composition for use in photochemical modeling. Figures 2-16 and 2-17 compare the reactive portions of the mean composition of the ambient samples to the compositions of the chamber mixtures, SynAuto and SynUrban. The compositions in the two tables are speciated for CAL and CB4, respectively. SynUrban is relatively close to the composition of the mean ambient mixture except that SynUrban contains a little more ethylene and lesser amounts of aldehydes than in the urban average. While the sigificance of this difference in terms of the production of ozone and formaldehyde should be investigated further, the reactivities of the SynUrban and mean ambient mixtures appear to be roughly equivalent.

Given that there is a range of levels of emissions that are possible from MFVs, particularly with future advances in technology, and a range of levels of usage or implementation, there is a range of emission mixtures which may be expected from large scale MFV usage.

Based on the measurements of Gold and Moulis [1987] and Snow, et al. [1989], the mixture of hydrocarbons emitted from MFVs meeting the current federal standards will be approximately 60% methanol and 5% formaldehyde with the balance being composed of the same hydrocarbons as emitted by gasoline fueled vehicles. If 100% of conventionally fueled vehicles were replaced by MFVs with these emissions, 65% of all motor vehicle hydrocarbon emissions (or 20 to 33% of all urban hydrocarbon emissions) would be replaced with a mixture of 92% methanol and 8% formaldehyde.

Under the California emissions standards, the percentage of formaldehyde and gasoline emissions from MFVs may drop to lower than 1%. If these advanced MFVs are used, a 33% replacement of total urban hydrocarbons would correspond to a replacement of 88% of conventionally fueled vehicles. If fewer conventionally fueled vehicles are replaced by MFVs, the actual replacement of total urban hydrocarbon emissions may be much lower than 20%.

While the conditions of the selected chamber experiments do not cover the full range of emisson mixtures that could be expected from the use of MFVs, the conditions are representative of the possible scenarios discussed above. Therefore, the chamber experiments do serve as adequate representations of the conditions that could be expected from large scale use of MFVs.

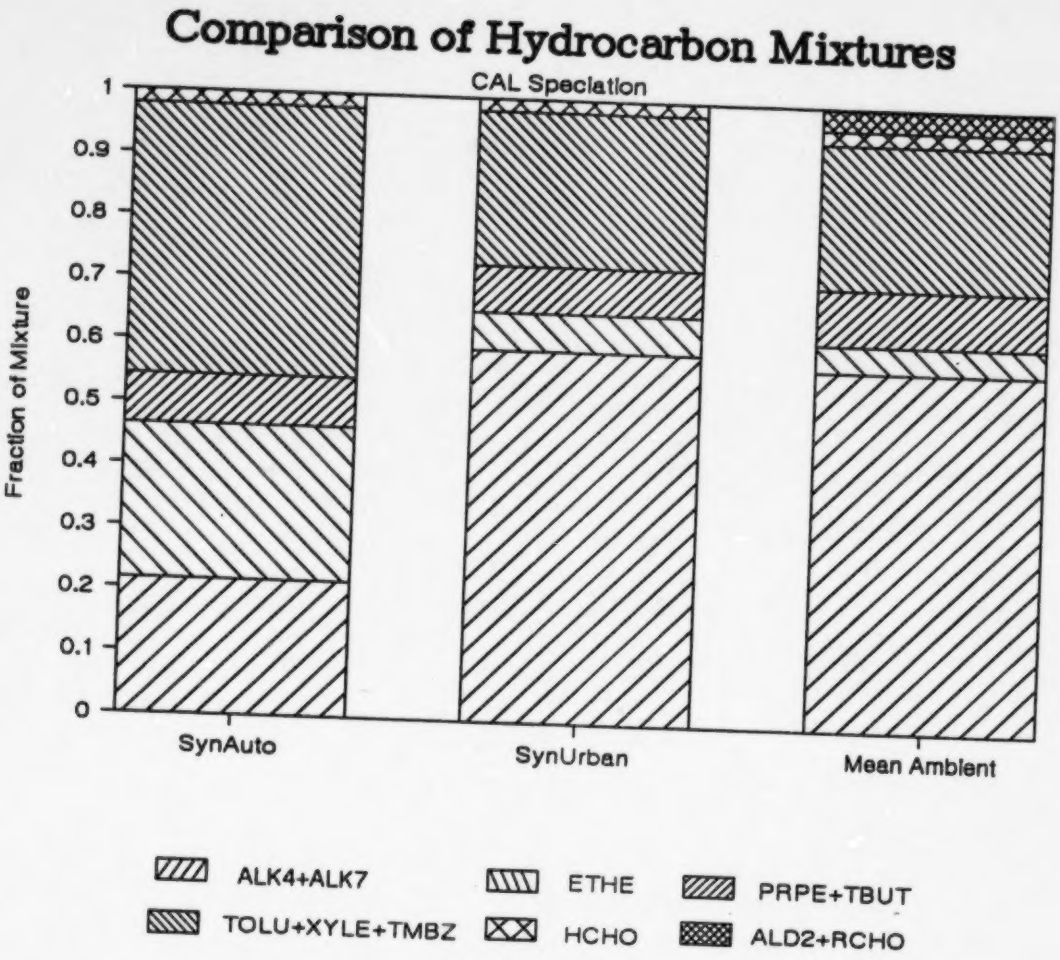

Figure 2-16. Comparison of Hydrocarbon Mixtures -CAL

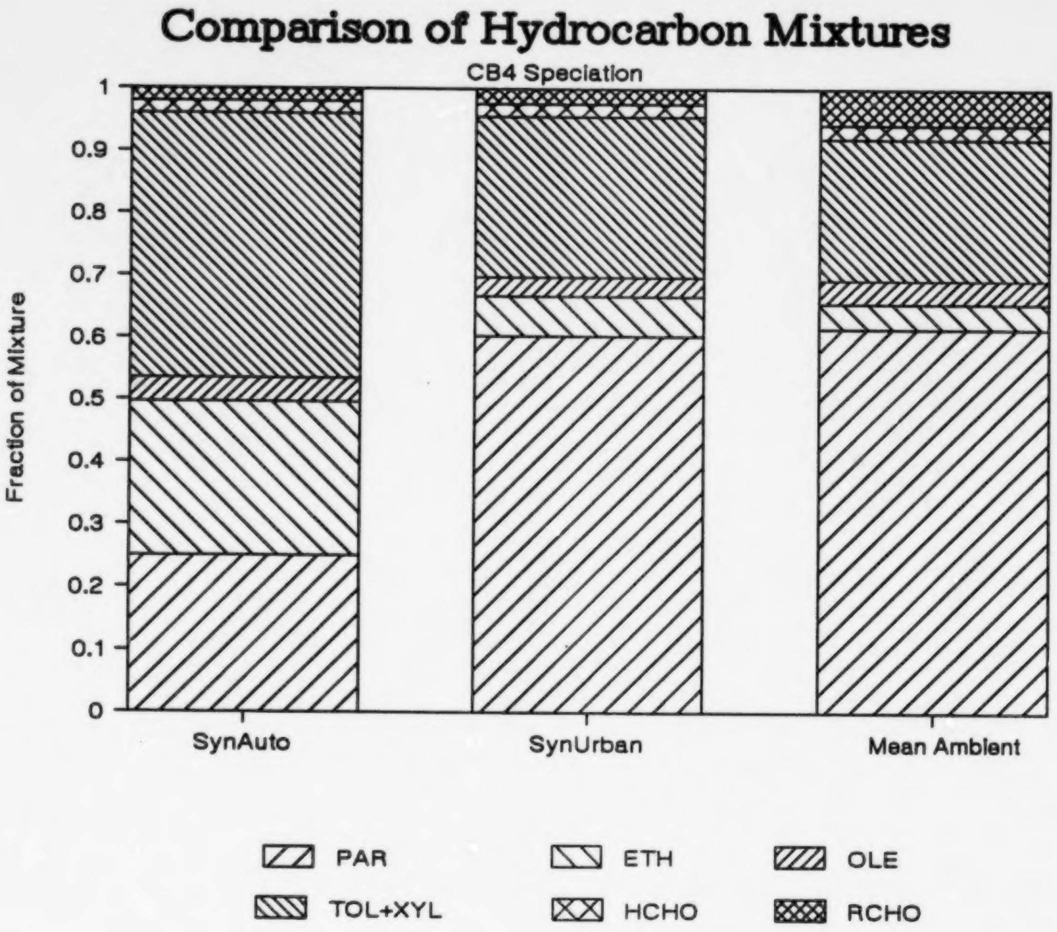

Figure 2-17. Comparison of Hydrocarbon Mixtures - CB4

Conclusions

The results of this evaluation may be summarized as follows:

Predictions of MFV Impacts

The performance of the mechanisms depends on the background mixture of hydrocarbons. If the SynUrban mixture is representative of the reactivity of the ambient hydrocarbon mixture, then CAL and CB4 would not not able to adequately predict the impacts of MFVs. Under such conditions, CAL and CB4 would be expected to over estimate the absolute concentrations of ozone and PAN and under estimate the absolute concentrations of formaldehyde. The relative changes predicted by the mechanisms would be expected to under estimate the ozone control benefits of MFV programs. If the ambient hydrocarbon mixture is more reactive than SynUrban, then CAL and CB4 may perform better in predicting both the absolute concentrations and relative changes resulting from MFV programs.

Overall, CAL and CB4 predict concentrations of ozone quite well. Their ability to predict formaldehyde concentrations is not as good, and their ability to predict PAN concentrations is quite poor. Currently, the ability to predict PAN concentrations is extremely sensitive to the assumptions made about wall processes.

In this evaluation, CIT did not perform as well as CAL and CB4, particularly in the late afternoon and under conditions of low hydrocarbon and NO_x concentrations. CIT over predicted the impacts of ozone and under predicted the impacts of formaldehyde and PAN. It is difficult to generalize from these results, however, because the available documentation for the mechanism does not provide enough information to confirm its proper implementation.

An effort should be made to measure definitively the methyl nitrite emissions from MFVs. If methyl nitrite is found not to be an artifact of the emission measurement process, its effect on formaldehyde concentrations should be evaluated using trajectory or grid-based models.

HCHO Control

The control of ambient levels of formaldehyde through selective control of ethylene emissions should be investigated in further smog chamber experiments and modeling exercises.

Future Utility of Current Models

In the future, I expect that the reactivity of ambient pollutant mixtures will decrease due to advances in technology and changes in public policy. In light of this expectation, the trend of decreasing mechanism performance with decreasing reactivity of the ambient hydrocarbon mixture raises doubt as to the utility of these state-of-the-art mechanisms in addressing future air quality concerns. Further smog chamber experimentation should be conducted to address the ablicability of current models to future pollutant mixtures.

As more information about the various effects of air pollutants is obtained, the appropriate measures of air quality will also change. These changes must be addressed in the model development and evaluation process if we are going to have useful tools for future decision making.

In the meantime, the use of mechanisms without adequate documentation should be strongly discouraged. Sexton and Jeffries [1987] have prepared an outline of an example guidance document which should be accepted as the standard for mechanism documentation.

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Methanol Fueled Vehicles and Photochemical Models:

An Evaluation of the State of Knowledge

Appendix A

By

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Department of Environmental Sciences and Engineering
School of Public Health
University of North Carolina, Chapel Hill

May, 1989

Sponsored By

The National Network for Environmental Management Studies
U.S. Environmental Protection Agency

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Appendix A

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Department of Environmental Sciences and Engineering
School of Public Health
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Appendix A

Individual Evaluations of Model Simulations

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September 21, 1984

Formaldehyde Addition

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June 26, 1985

1/3 Hydrocarbon Reduction

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June 28, 1985

1/3 Methanol Substitution w/10% HCHO

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August 4, 1984: 1/3 Methanol Substitution w/10% HCHO

Top: 1.25 ppmC SynAuto
Bottom: 0.83 ppmC SynAuto, 0.3 ppm MEOH, 0.03 ppmC HCHO

Chamber Observations:

In Figure A1, note that the temperature is below the dewpoint suggesting that condensation may have occured on the chamber walls. Given this condensation, the timing of the model predictions is expected to be late in comparison to the timing of observed events. The methanol substitution reduced the peak concentration of ozone from about 0.5 ppm to about 0.3 ppm.

CB4 and CAL Predictions:

As expected, the NO_x crossover points (Fig. A2) and hydrocarbon decay profiles (Fig. A3) predicted by CB4 and CAL are shifted to the right of the observed events. The methanol decay profiles predicted by CB4 and CAL are identical but are much slower than the observed decay profile.

CB4 and CAL over predict the ozone concentration profiles (Fig. A2) on the control side (top) with P/O ratios of 1.3 and 1.2, respectively. The over prediction is greater on the substitution side (bottom), and therefore, the relative change in ozone concentrations due to the methanol substitution is under predicted by the mechanisms.

In Figure A4, CB4 and CAL predict formaldehyde concentrations which are twice the observed concentrations on both sides of the chamber. CAL over predicts PAN concentrations, but the predictions of CB4 are adequate.

Wall Model Effects:

Switching to Killus's wall model (Figs. A5-7) improves ozone and PAN predictions but has no effect on formaldehyde predictions. Removing the wall reactions (Figs. A8-10) causes CB4 and CAL to under predict the concentrations of ozone and PAN and decreases the over prediction of formaldehyde.

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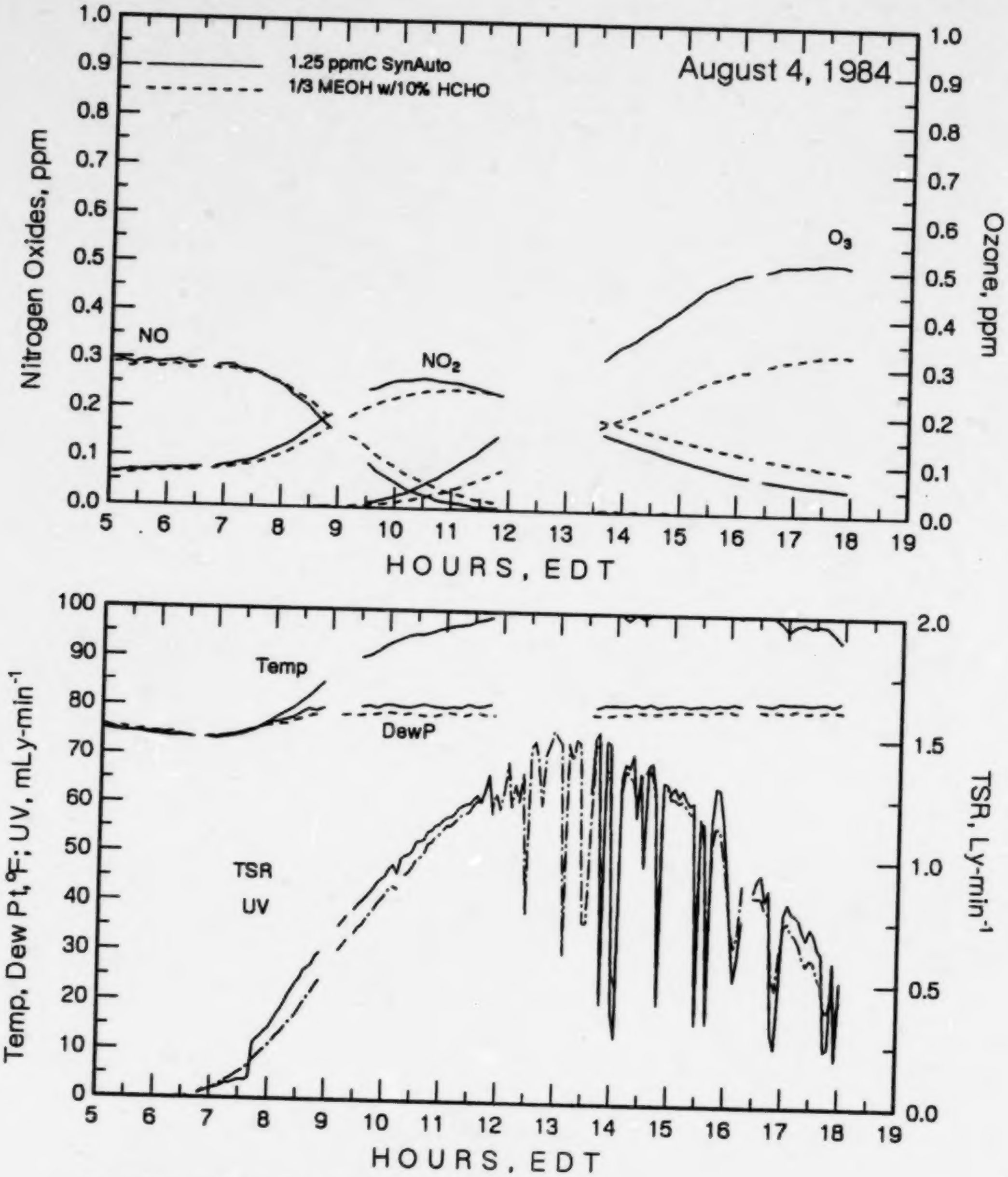
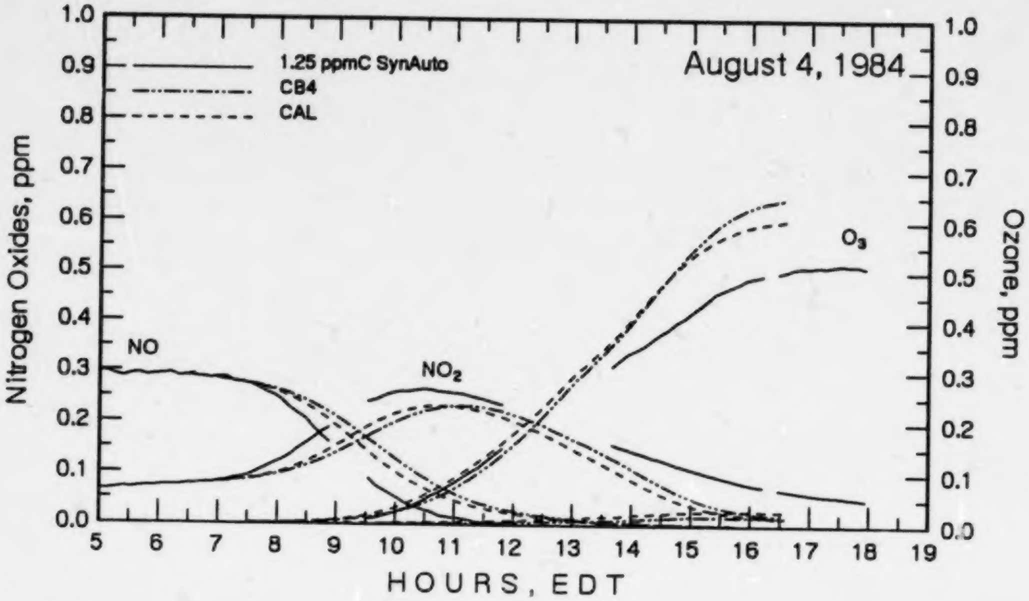


Figure A1. Chamber Observations.



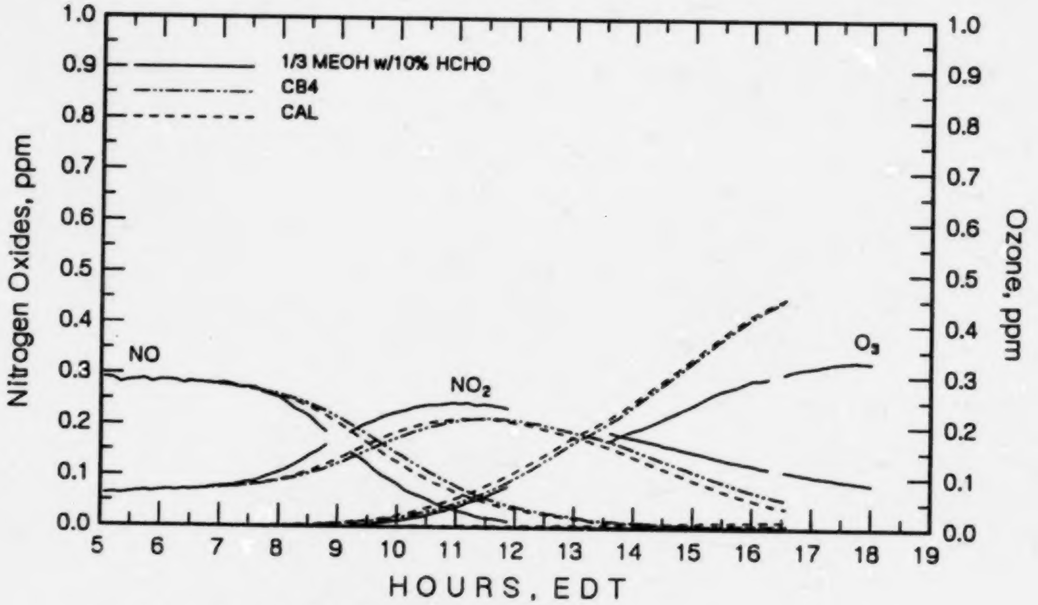


Figure A2. CB4 and CAL Predictions.

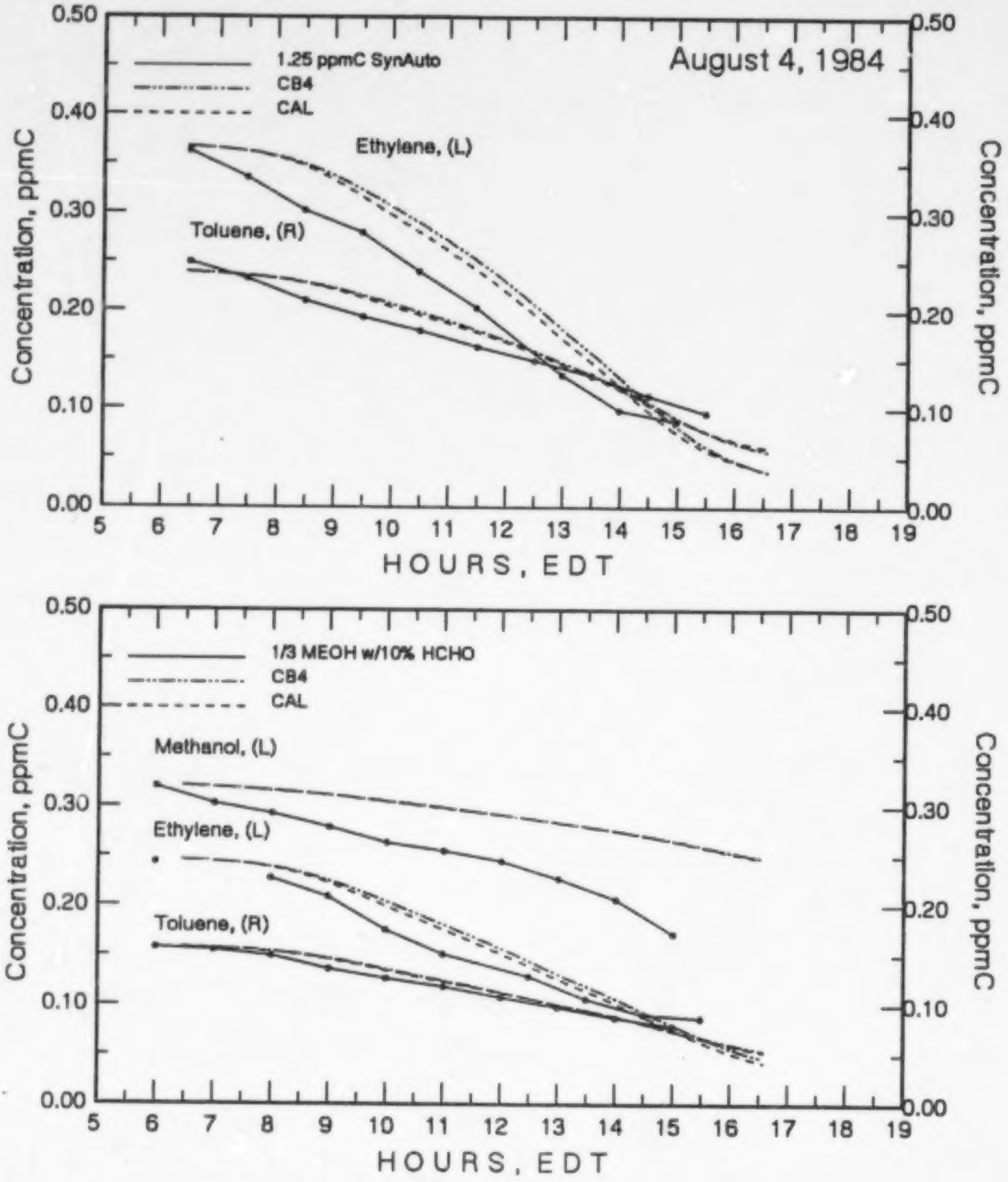


Figure A3. CB4 and CAL Predictions.

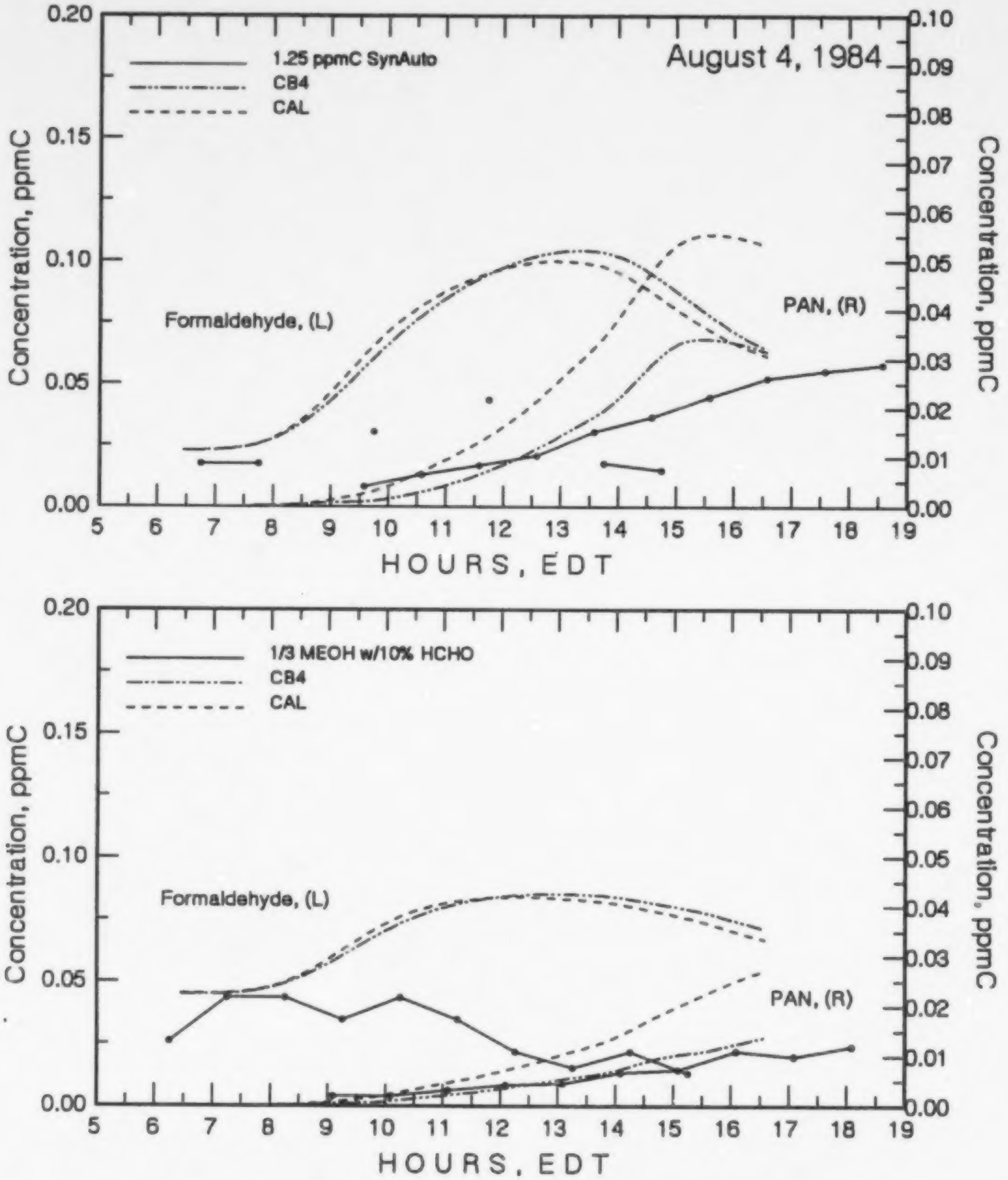


Figure A4. CB4 and CAL Predictions.

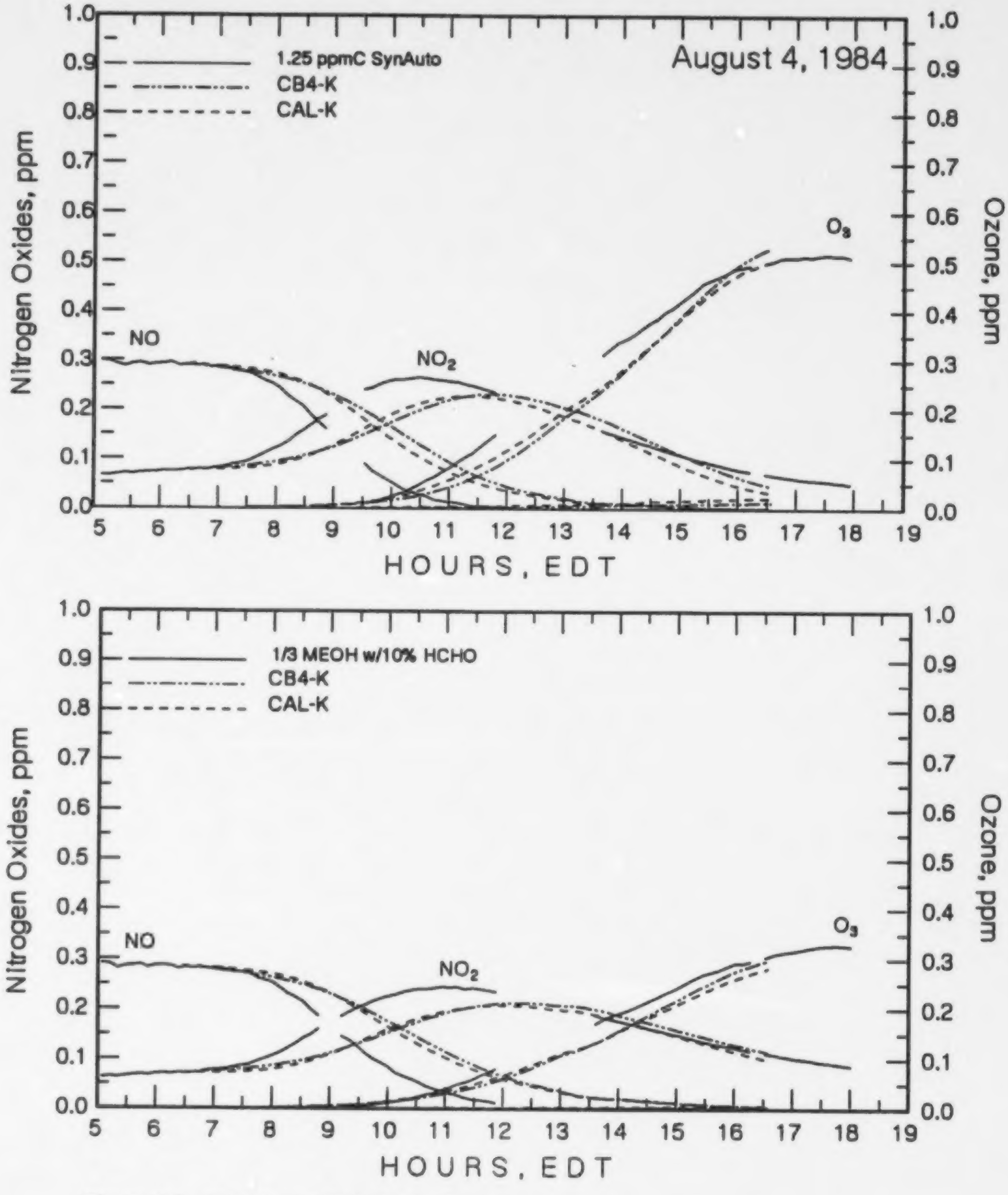


Figure A5. CB4-K and CAL-K Predictions.

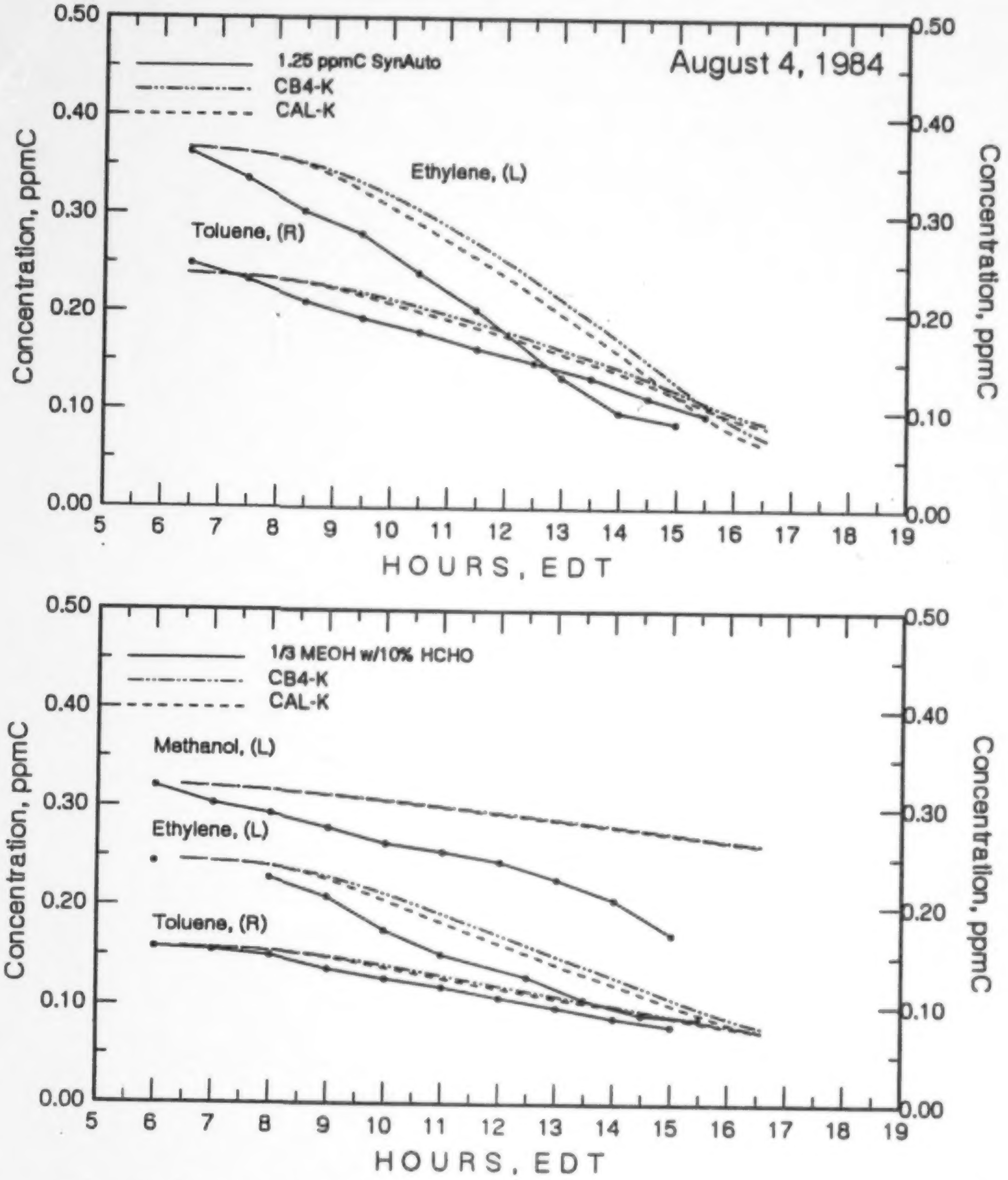
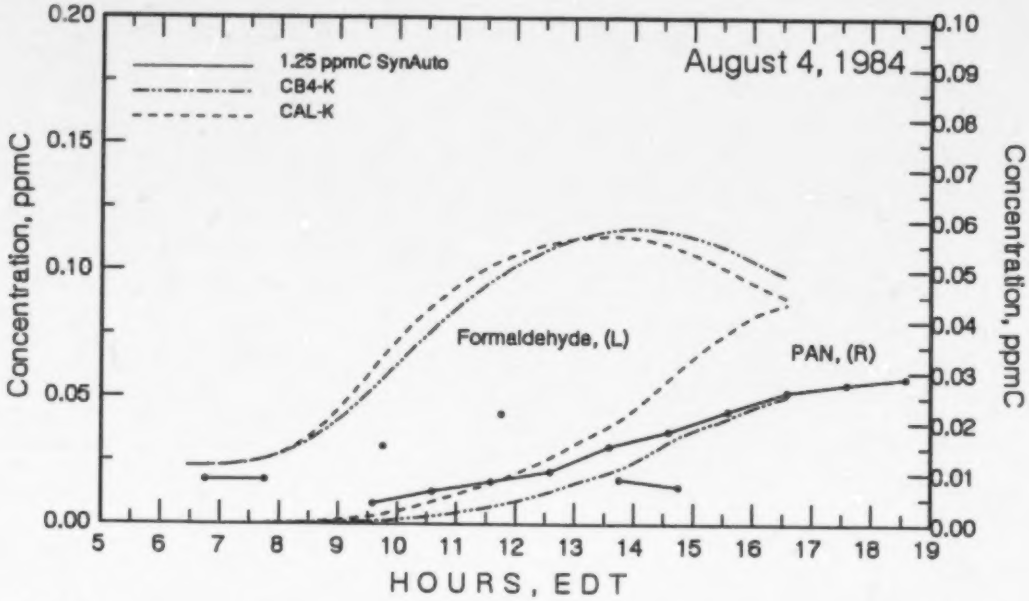


Figure A6. CB4-K and CAL-K Predictions.



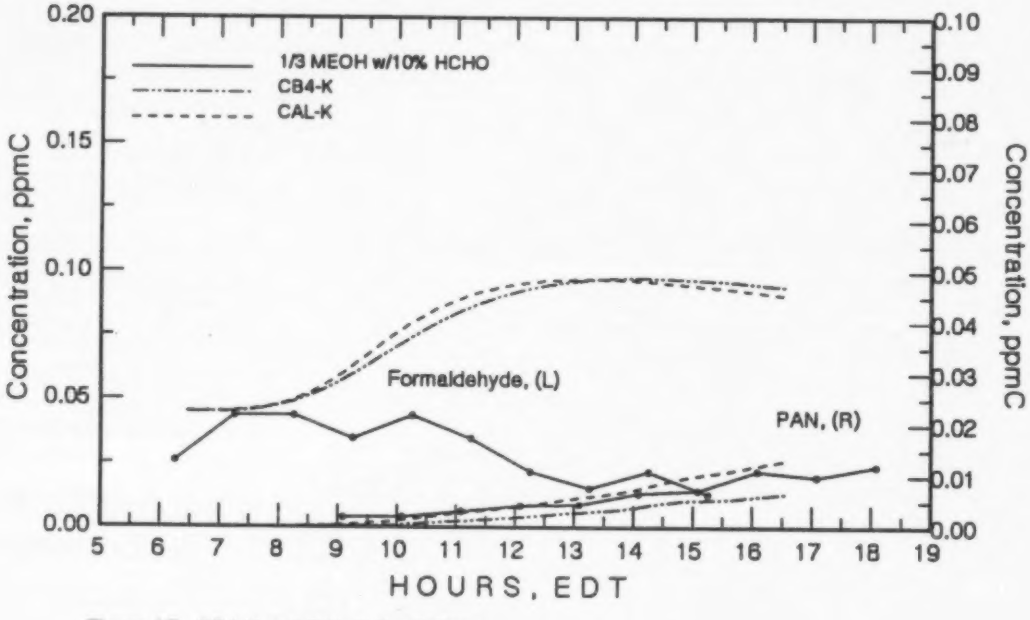
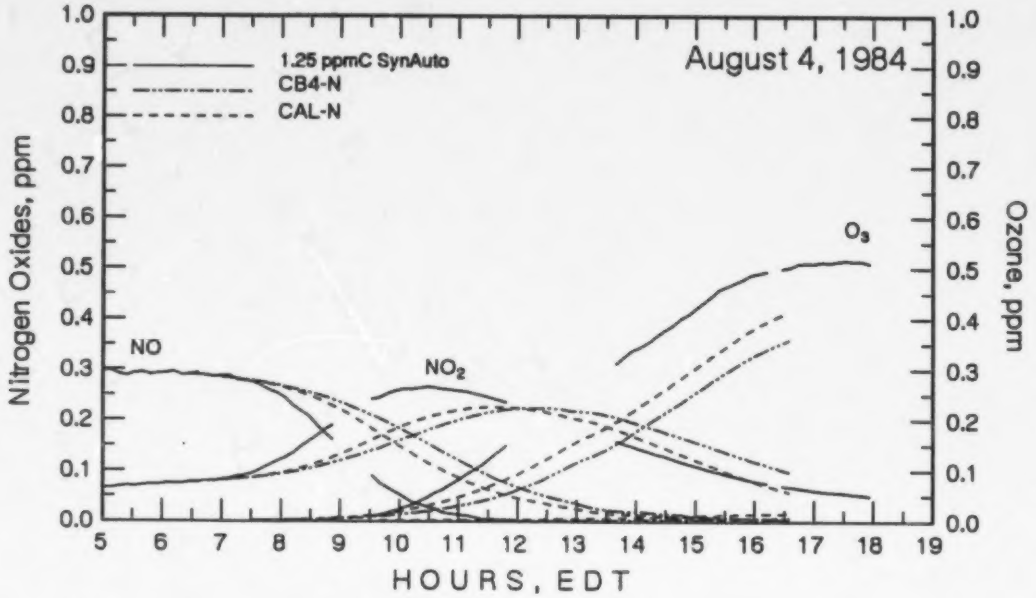


Figure A7. CB4-K and CAL-K Predictions.



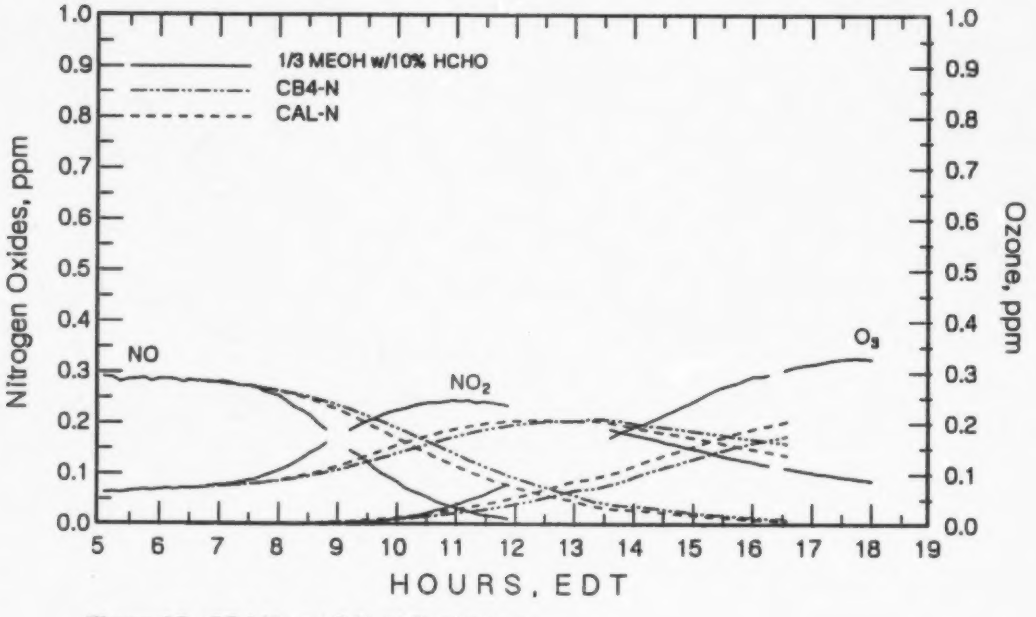


Figure A8. CB4-N and CAL-N Predictions.

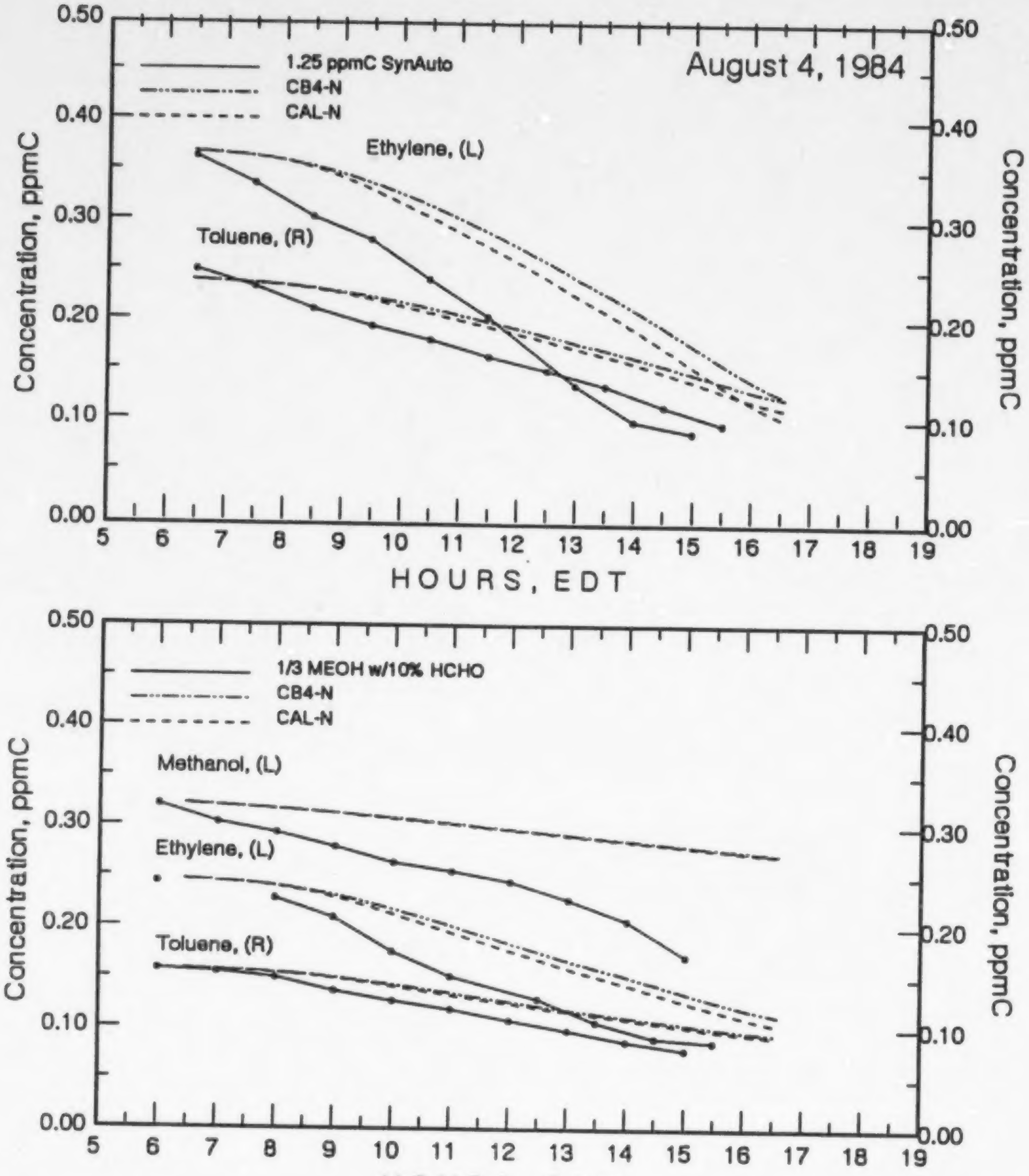


Figure A9. CB4-N and CAL-N Predictions.

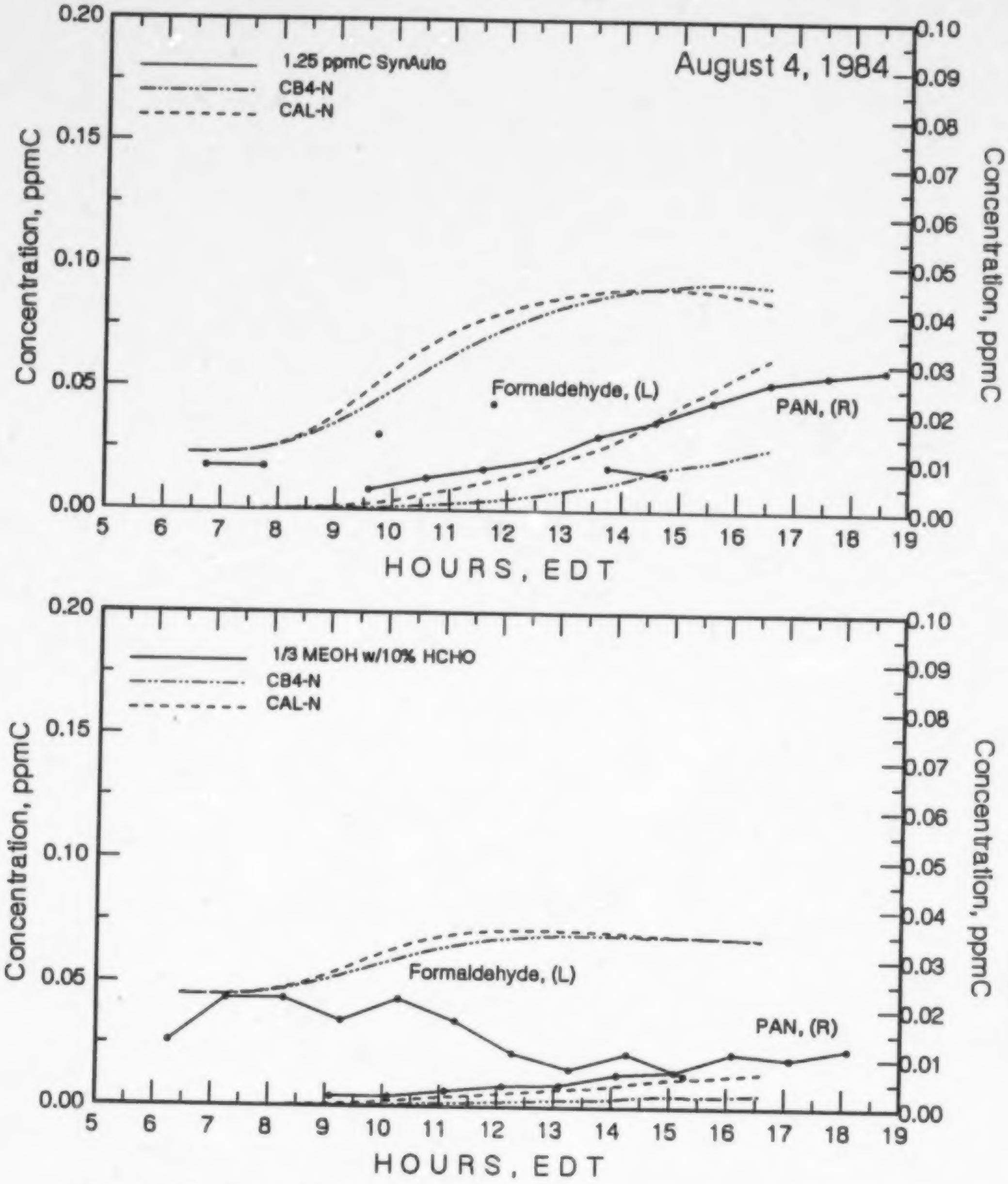


Figure A10. CB4-N and CAL-N Predictions.

August 5, 1984: 1/3 Hydrocarbon Reduction

Top: 0.93 ppmC SynAuto
Bottom: 1.33 ppmC SynAuto

Chamber Observations:

During the early morning hours, the temperature (Fig. A11) is below the dewpoint; therefore, the model predictions are expected to be late. The reduction of initial hydrocarbon produced a decrease in peak ozone concentration from approxiamately 0.6 ppm to approxiamately 0.3 ppm.

CB4 and CAL Predictions:

As expected the NO_x crossover points (Fig. A12) predicted by CB4 and CAL are later than the observed points on both sides of the chamber.

Given the timing problem, the toluene decay profiles (Fig. A13) predicted by CB4 and CAL are too early. The predicted ethylene decay profiles are actually correct, except that the decay profiles predicted for the control side (bottom) are faster than the observed decay profile at the end of the day.

The ozone concentration profiles (Fig. A12) predicted by CB4 and CAL appear to agree with the observed concentrations on both sides of the chamber. Relative to the predicted timing of the NO_x crossover point, however, the ozone predictions are too early and over predict the observed ozone concentrations. This over prediction appears to be the same on both sides of the chamber, and therefore, the relative change in ozone concentrations due to the reduction of initial hydrocarbons is predicted well by both CB4 and CAL.

The PAN concentrations (Fig. A14) predicted by CB4 for the reduction side (top) agree with the observed concentrations. On the control side (bottom), CB4 over predicts the peak PAN concentration with a P/O ratio of 1.4. CAL over predicts the PAN concentrations on both sides of the chamber with P/O ratios greater than 2. The formaldehyde concentrations predicted by CB4 and CAL agree with the observed concentrations on both sides of the chamber. There is a problem in the observed formaldehyde concentrations for this experiment, however, caused by water condensation in the chamber sampling line.

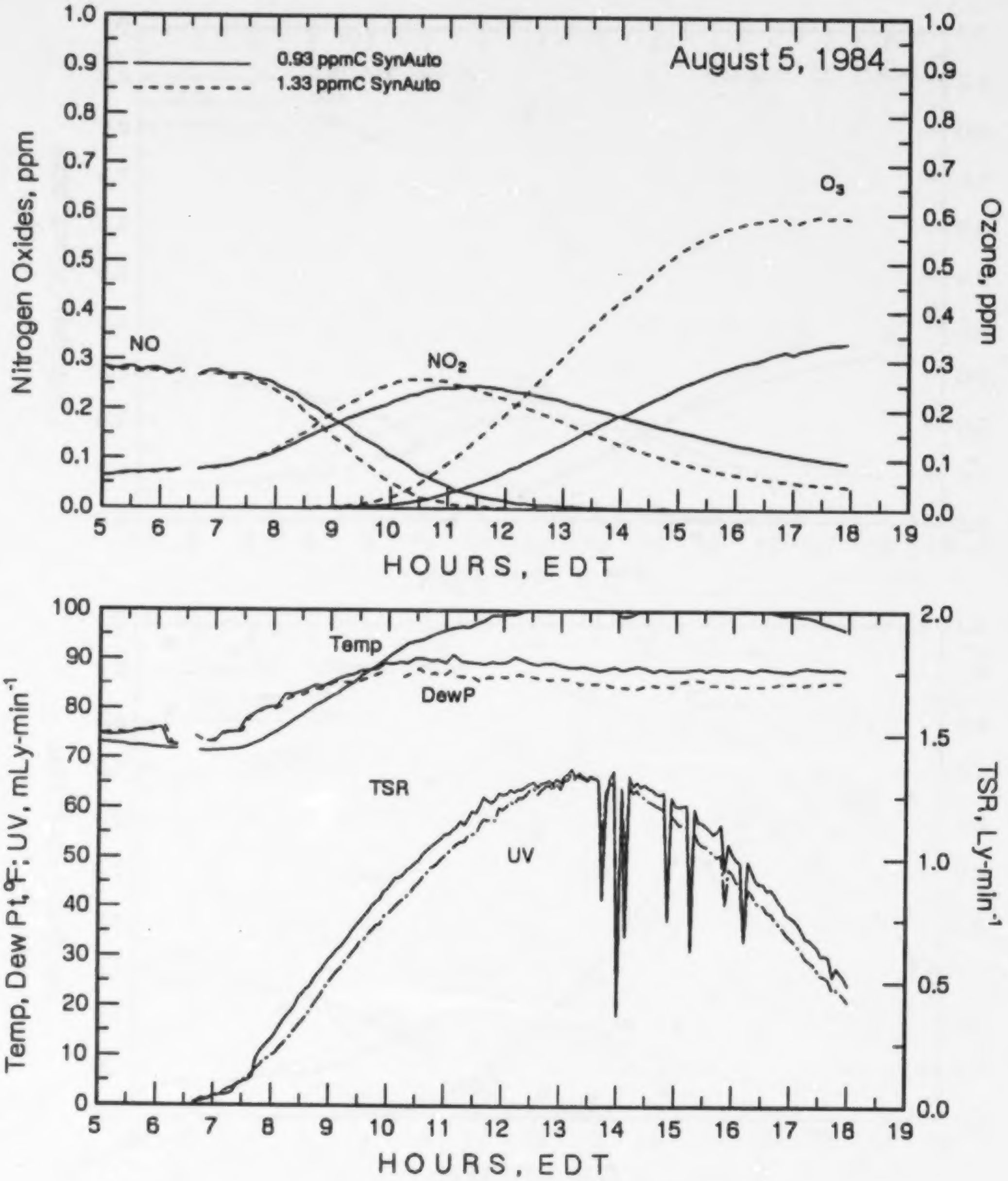


Figure A11. Chamber Observations.

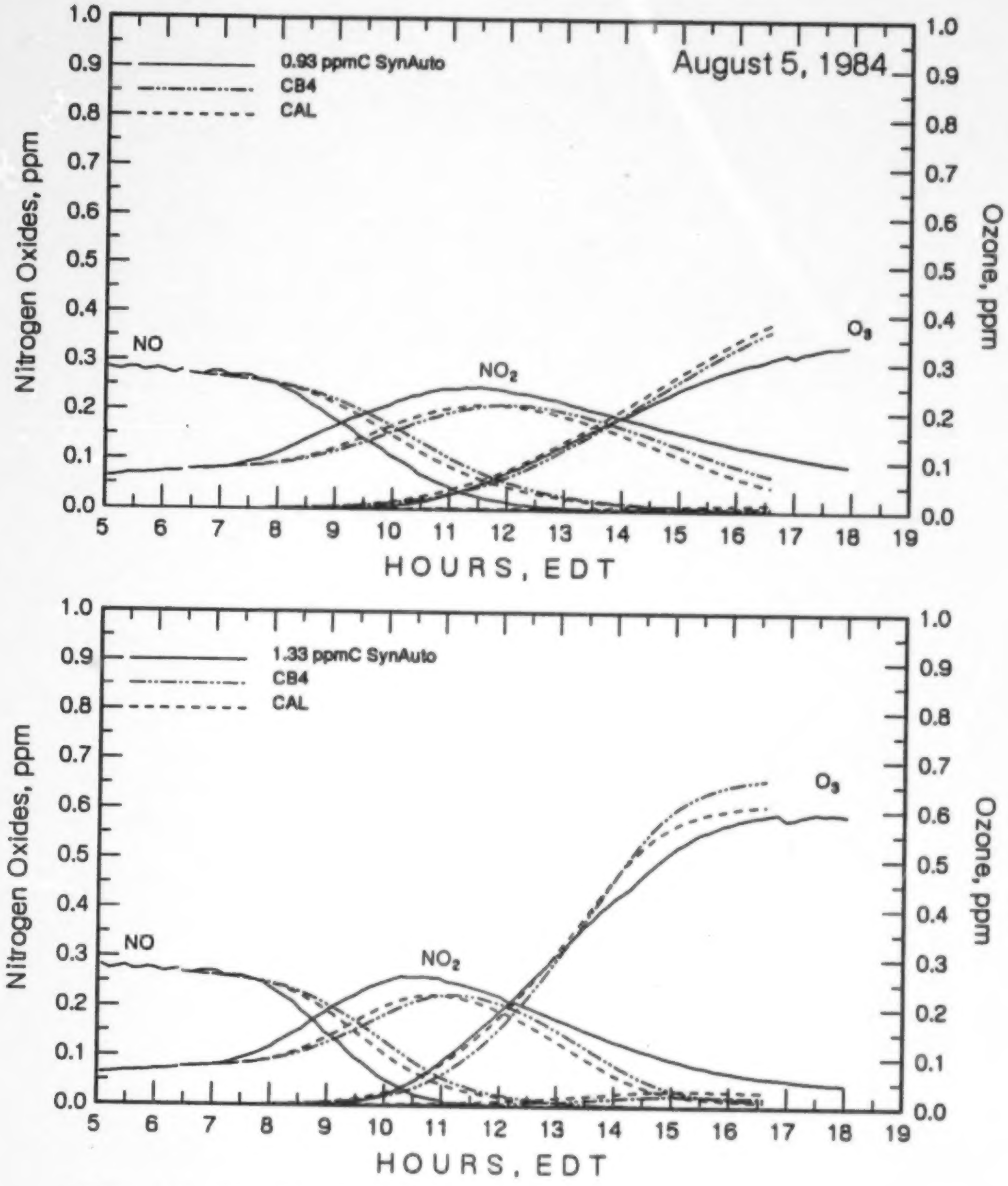


Figure A12. CB4 and CAL Predictions.

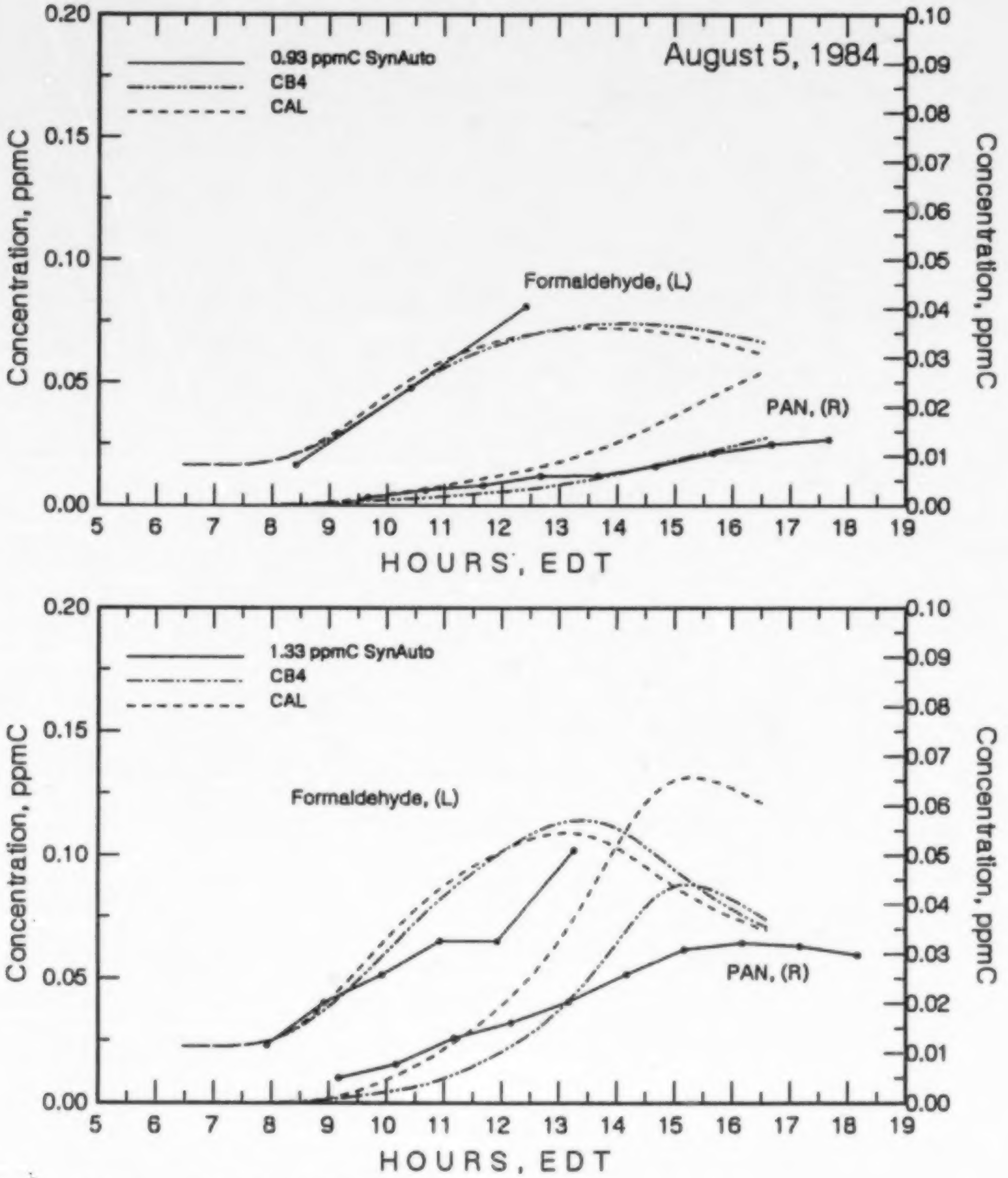


Figure A14. CB4 and CAL Predictions.

August 8, 1984: 1/3 Hydrocarbon Reduction

Top: 2.29 ppmC SynAuto
Bottom: 3.29 ppmC SynAuto

Chamber Observations:

The temperature (Fig. A15) is below the dewpoint in the early morning hours of the experiment; thus, the model predictions are expected to be late in comparison to the observed data. Although one third of the initial hydrocarbon was removed, there was very little change in the peak concentration of ozone.

CB4 and CAL Predictions:

As expected, the predicted NO_x crossover points (Fig. A16) are late compared to the observed crossover points.

Taking into account the timing problem, the hydrocarbon decay (Fig. A17) and the ozone production profiles (Fig. A16) predicted by CB4 and CAL agree with the observed profiles.

The formaldehyde concentrations (Fig. A18) predicted by CB4 and CAL for the reduction side (top) agree well with the observed concentrations. On the control side (bottom), the models over predict the formaldehyde concentrations. There are no observations of PAN concentrations for this experiment.

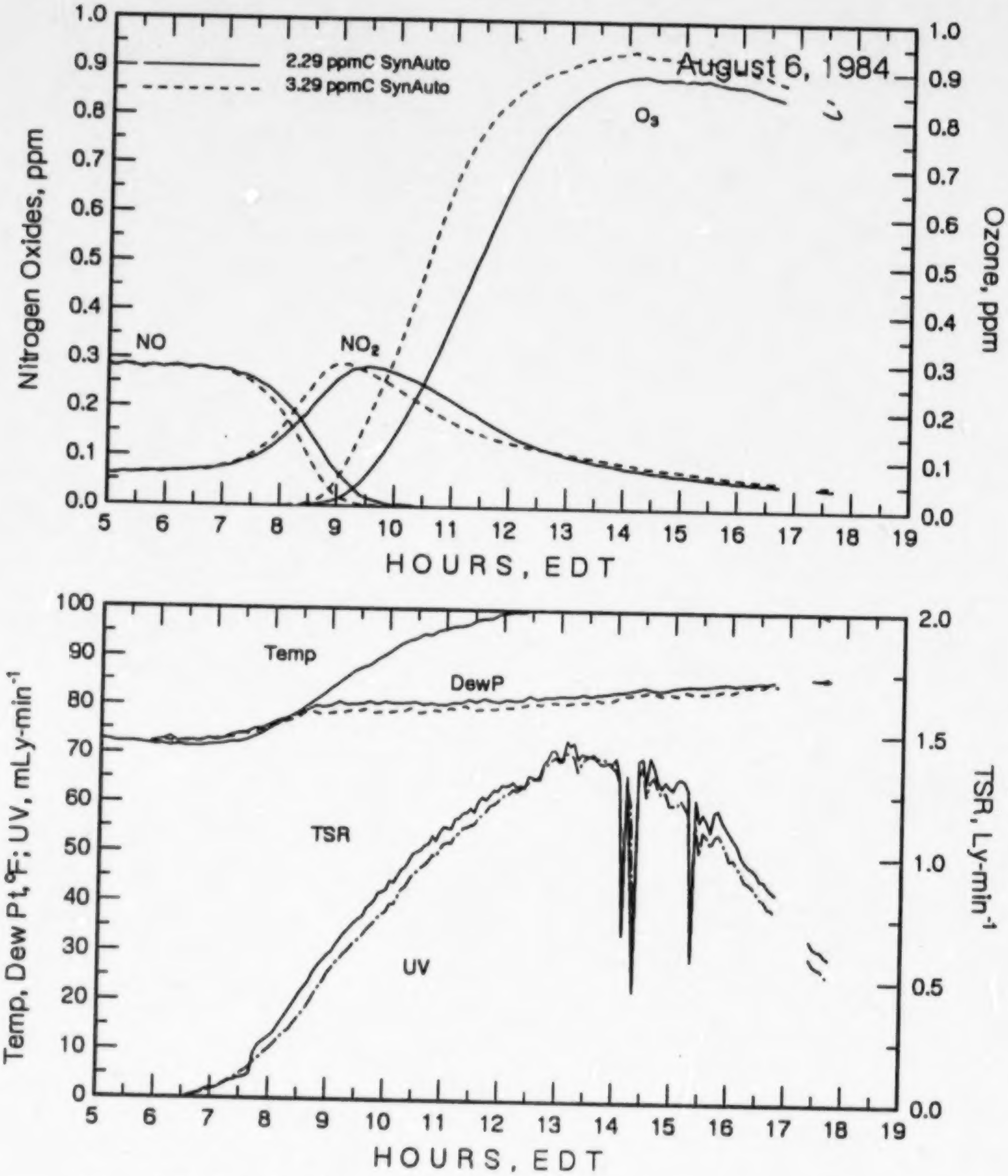


Figure A15. Chamber Observations.

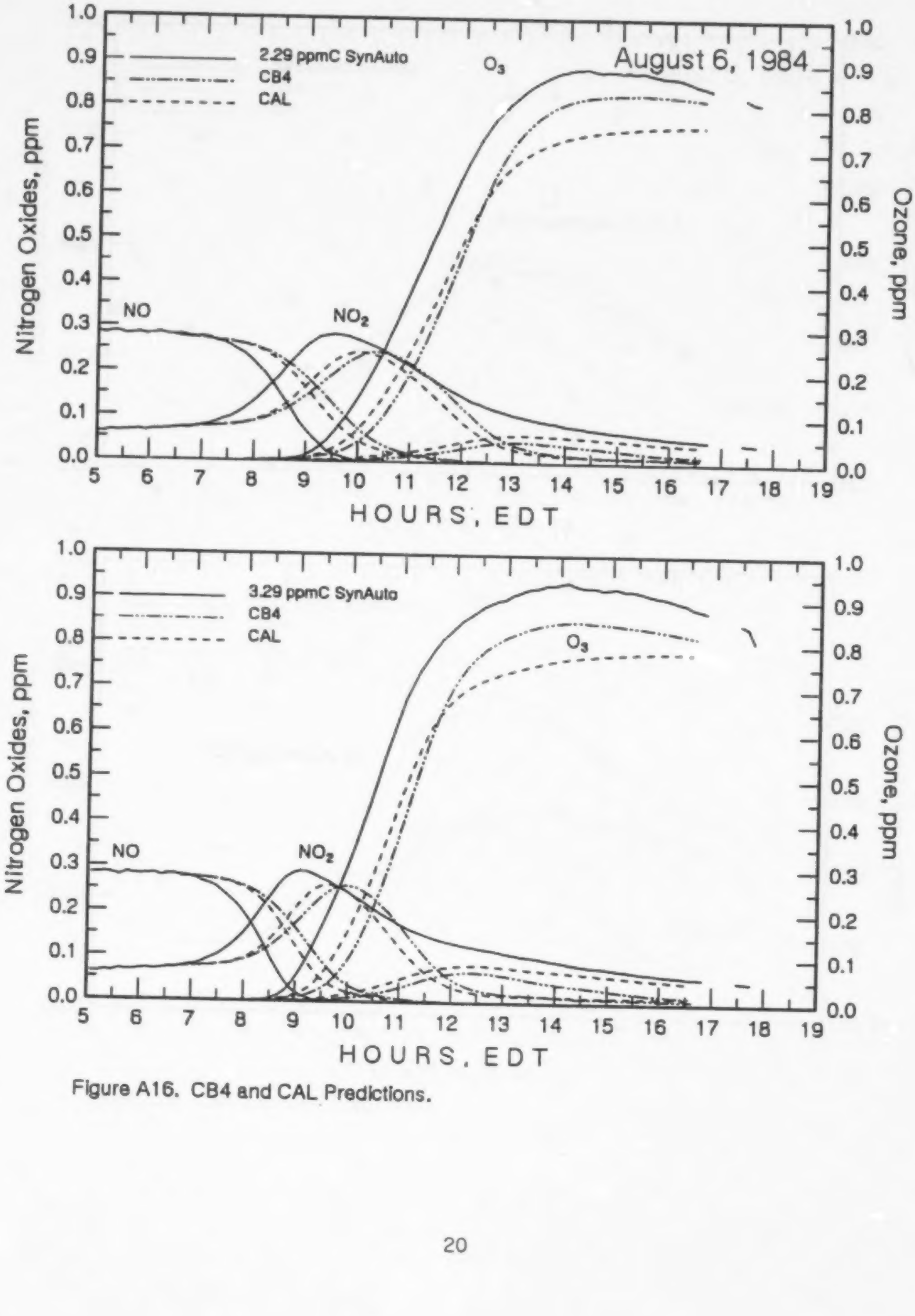

August 6, 1984

Figure A16. CB4 and CAL Predictions.

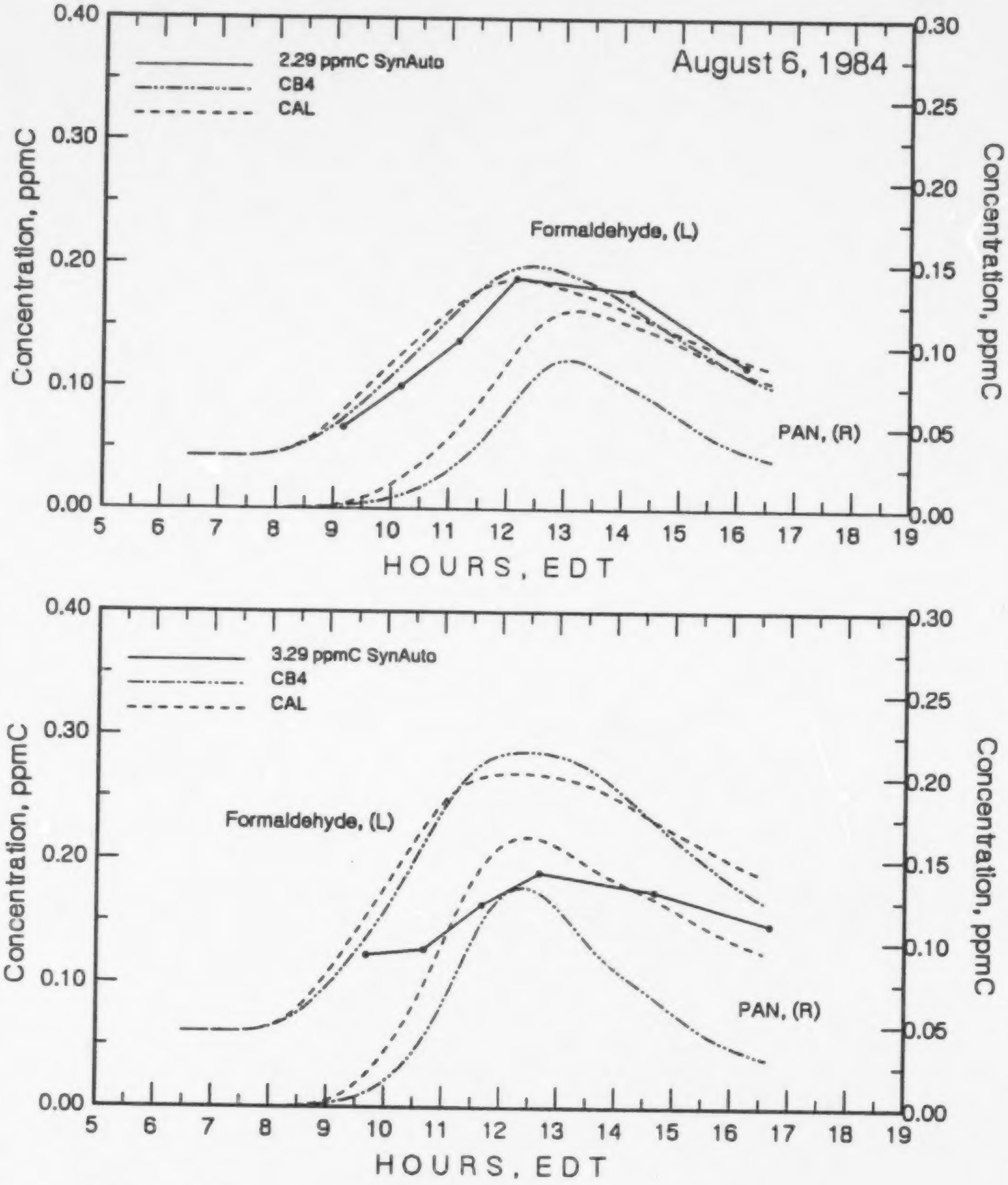


Figure A18. CB4 and CAL Predictions.

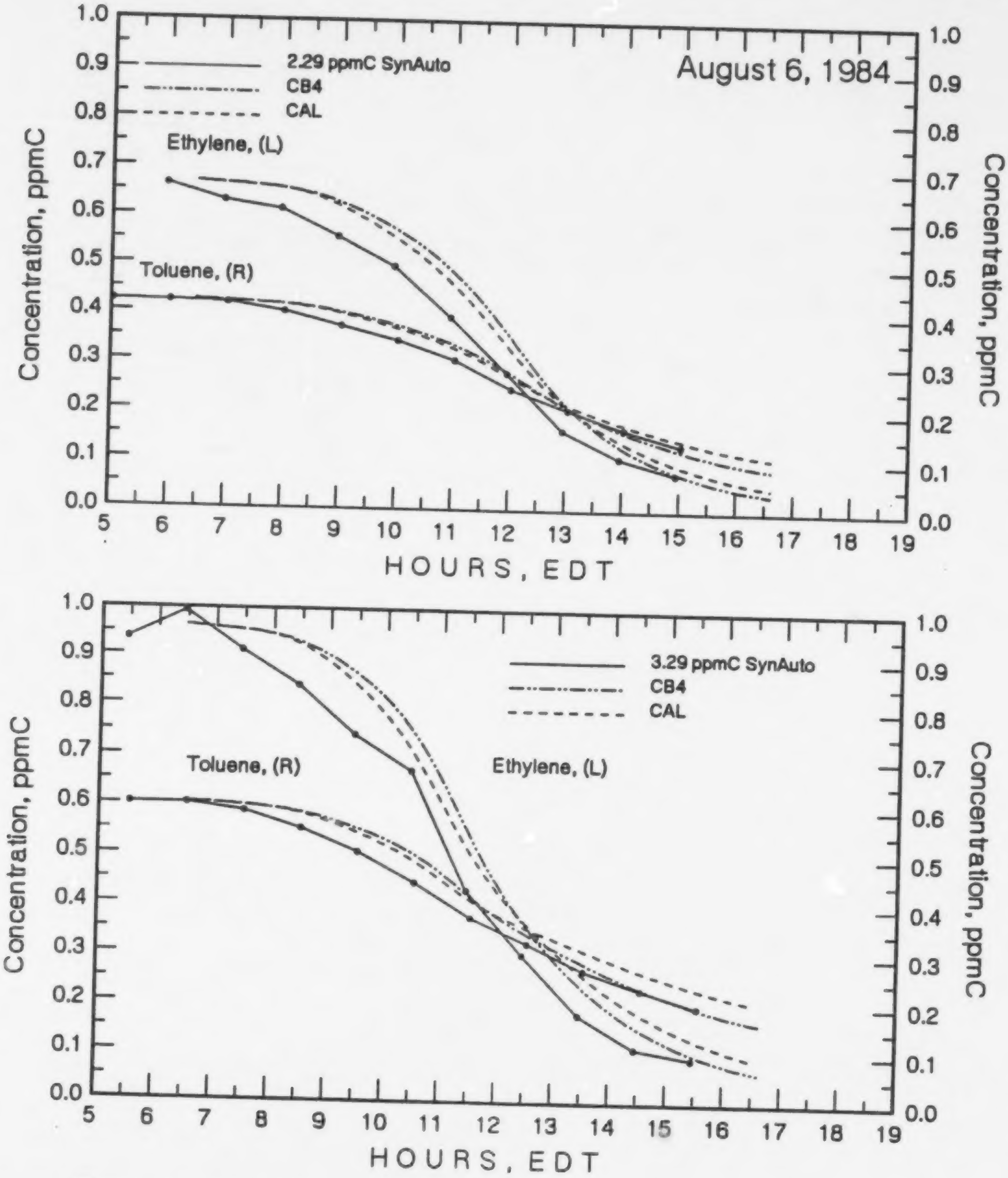


Figure A17. CB4 and CAL Predictions.

August 7, 1984: 1/3 Methanol Substitution

Top: 1.36 ppmC SynAuto
Bottom: 0.89 ppmC SynAuto, 0.3 ppm MEOH, 0.03 ppm HCHO

Chamber Observations:

There are no temperature observations (Fig. A19) for the early morning hours of this experiment, but most likely there was condensation and a timing problem should be expected. The methanol substitution resulted in a reduction in the peak ozone concentration from approxiamately 0.6 ppm to 0.4 ppm.

CB4 and CAL Predictions:

As expected, the NO_x crossover points (Fig. A20) and the hydrocarbon decay profiles (Fig. A21) are late compared to the observed data.

There is a discrepancy between the reported initial concentrations of methanol, which were used in the simulations, and the observed concentrations (Fig. A21).

The predicted ozone concentrations (Fig. A20) agree well with the observed concentrations on both sides of the chamber. Given the timing problems, however, the models actually over predict the ozone concentrations.

Considering the timing problems, the formaldehyde concentration profiles (Fig. A22) predicted by CB4 and CAL agree with the observed profiles. While CB4 predicts PAN concentrations correctly, CAL over predicts the PAN concentrations with P/O ratios equal to approxiamately 2 on both sides of the chamber.

Addition of Methyl Nitrite:

Explicitly accounting for the presence of methyl nitrite (Figs. A23-5) shifts the predicted formaldehyde profile to the left.

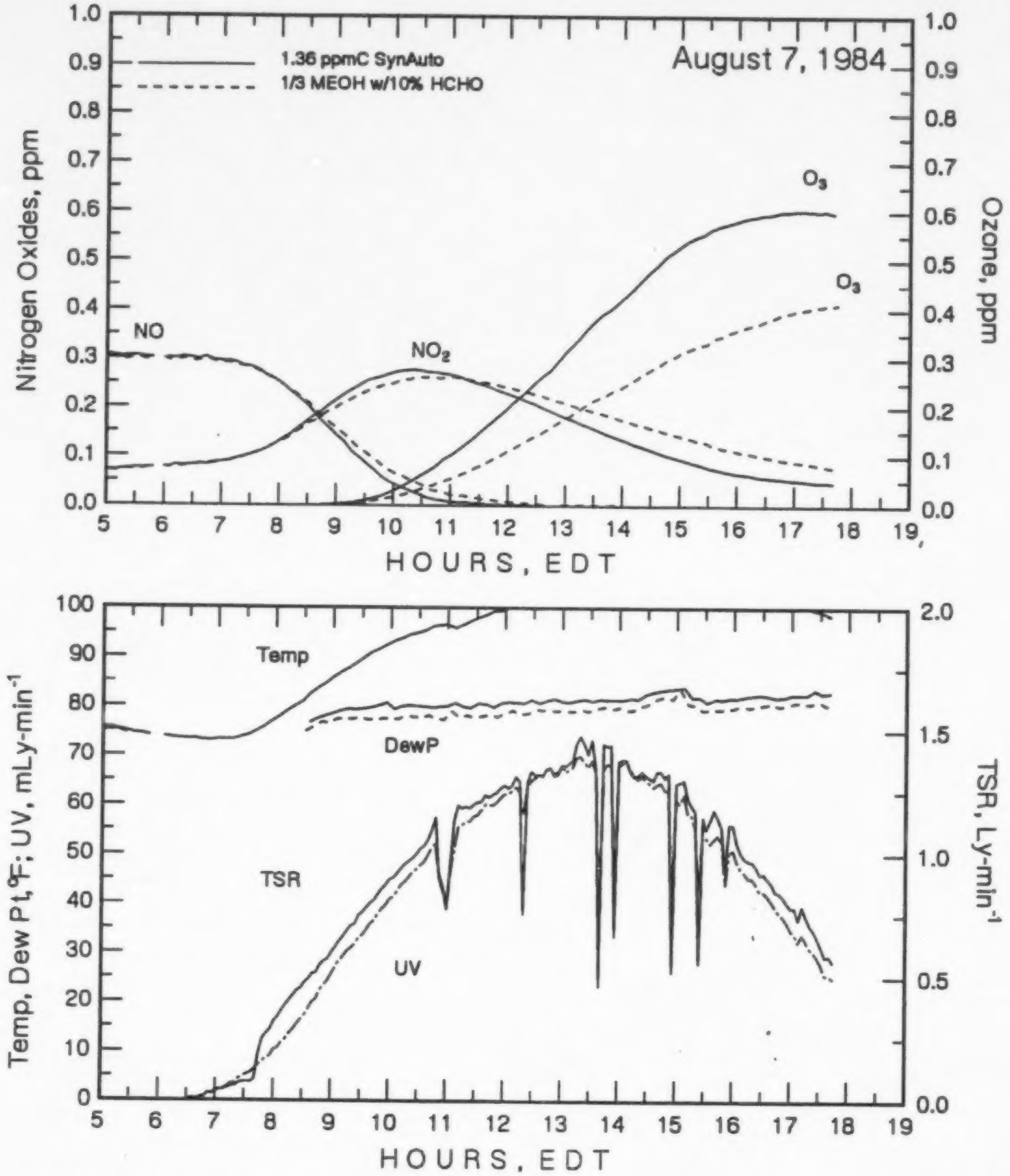


Figure A19. Chamber Observations.

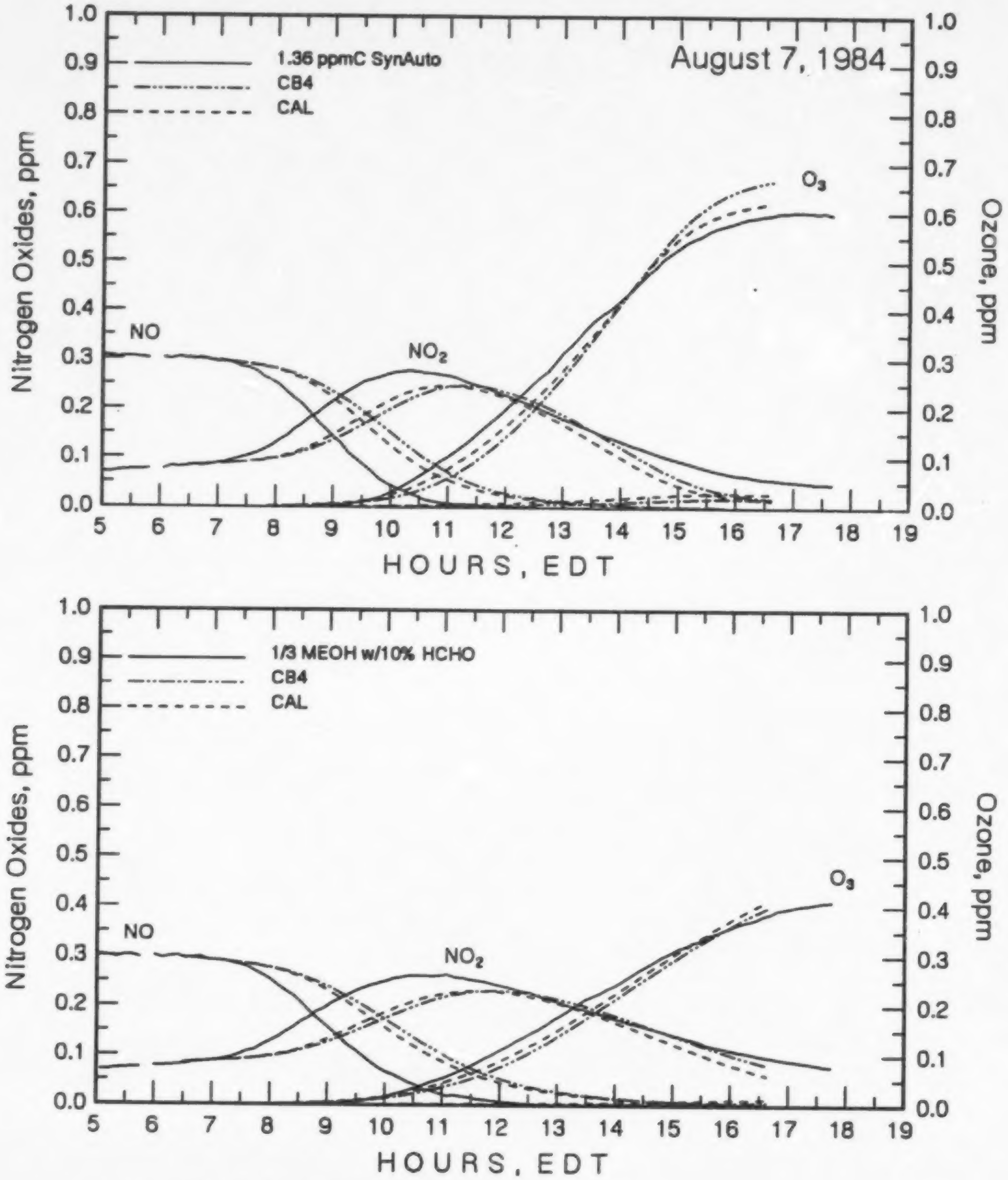
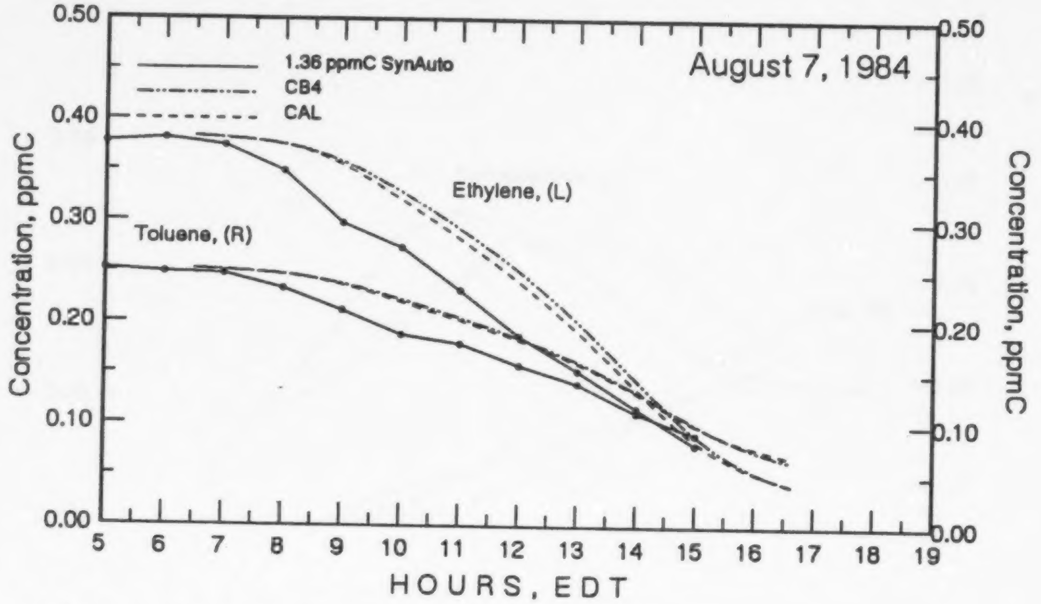


Figure A20. CB4 and CAL Predictions.



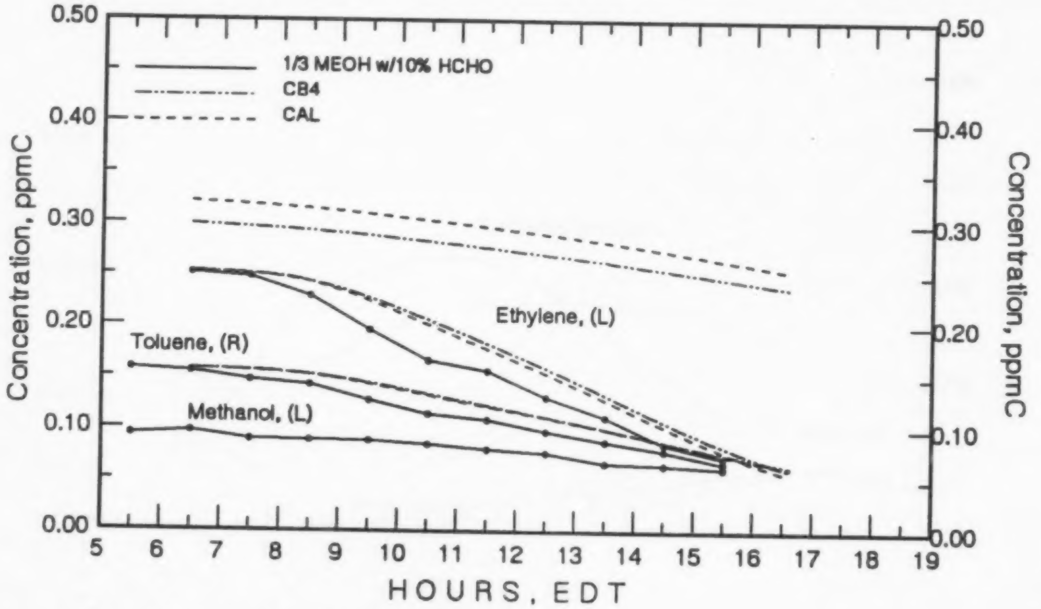


Figure A21. CB4 and CAL Predictions.

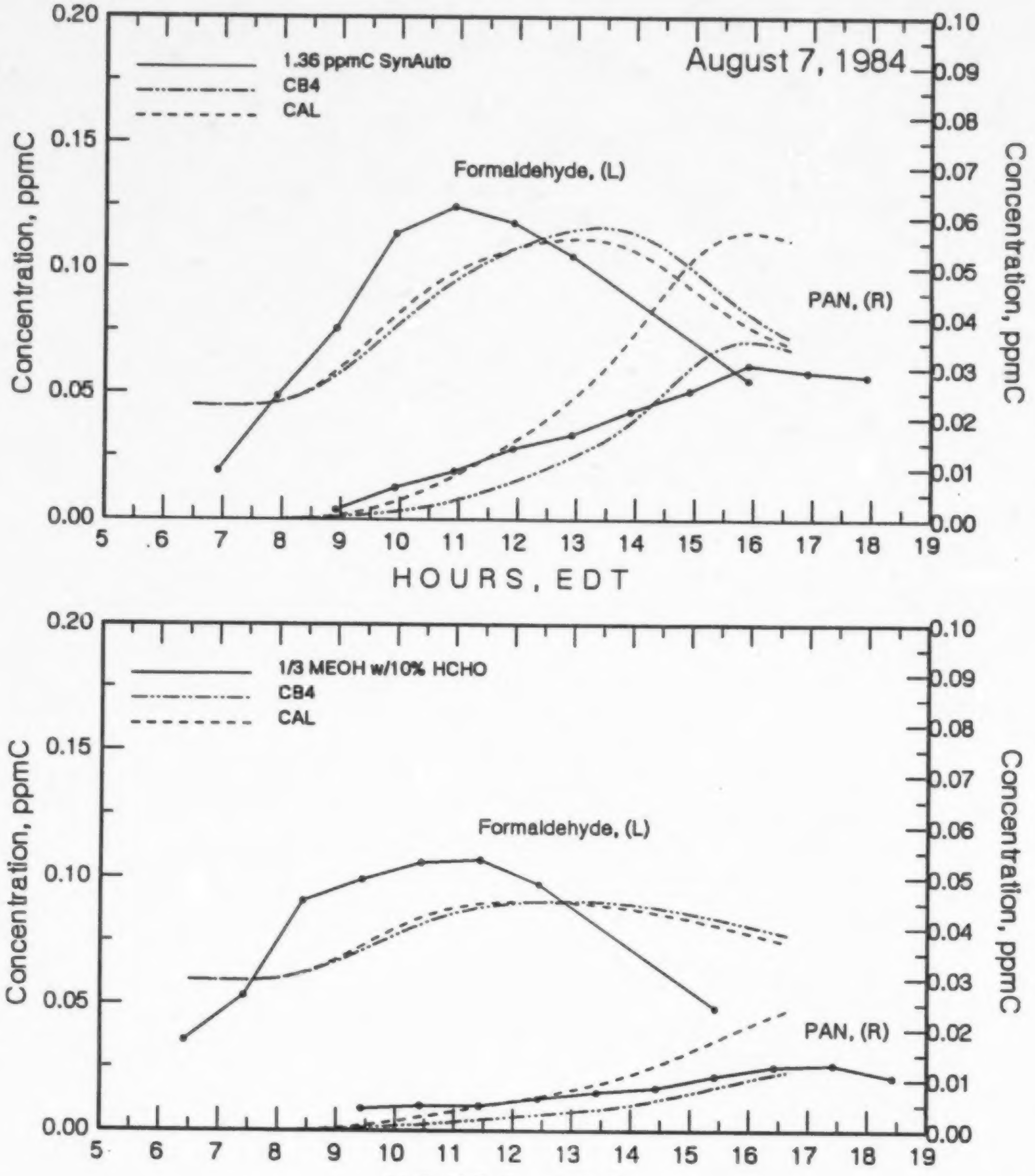


Figure A22. CB4 and CAL Predictions.

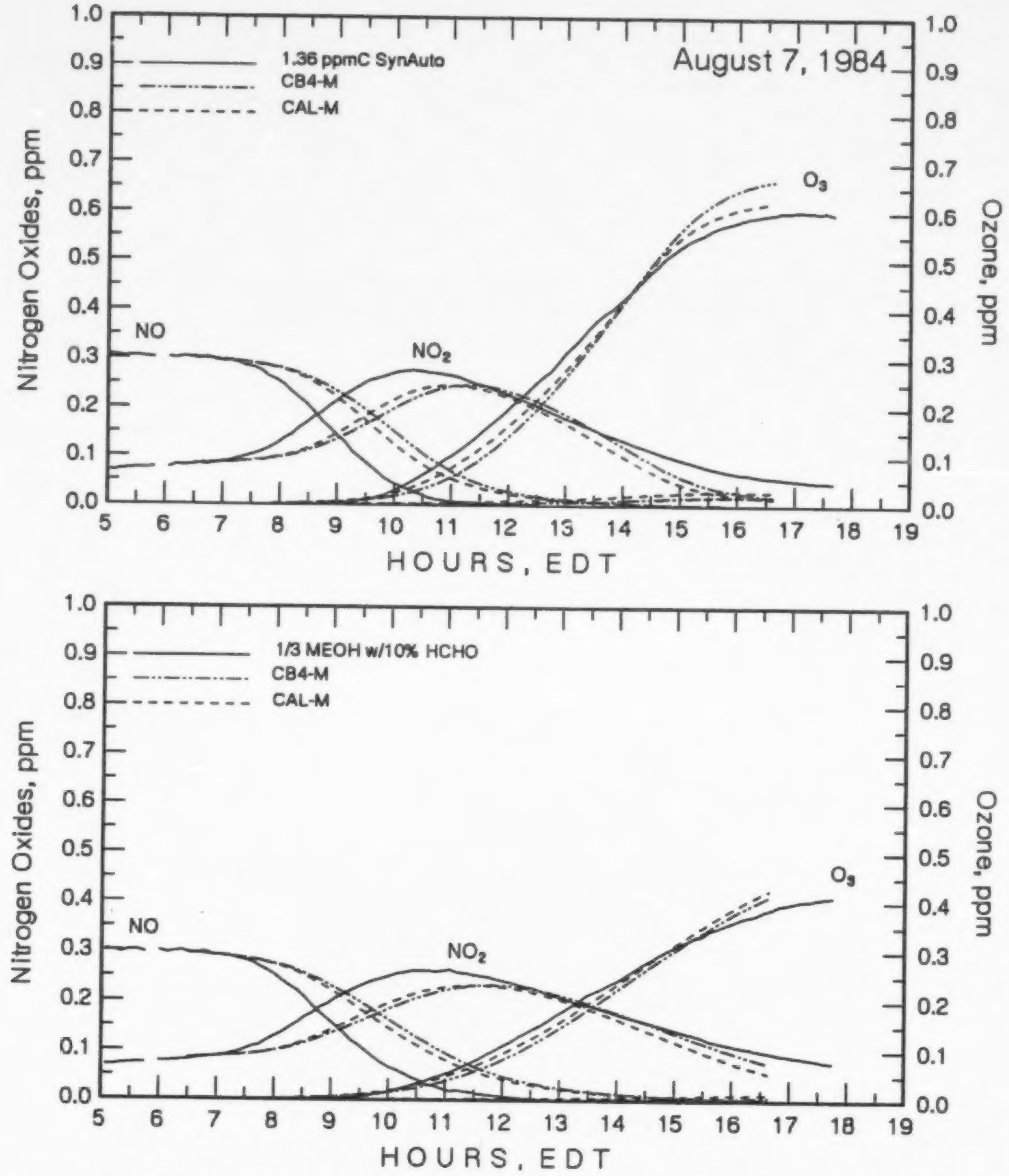
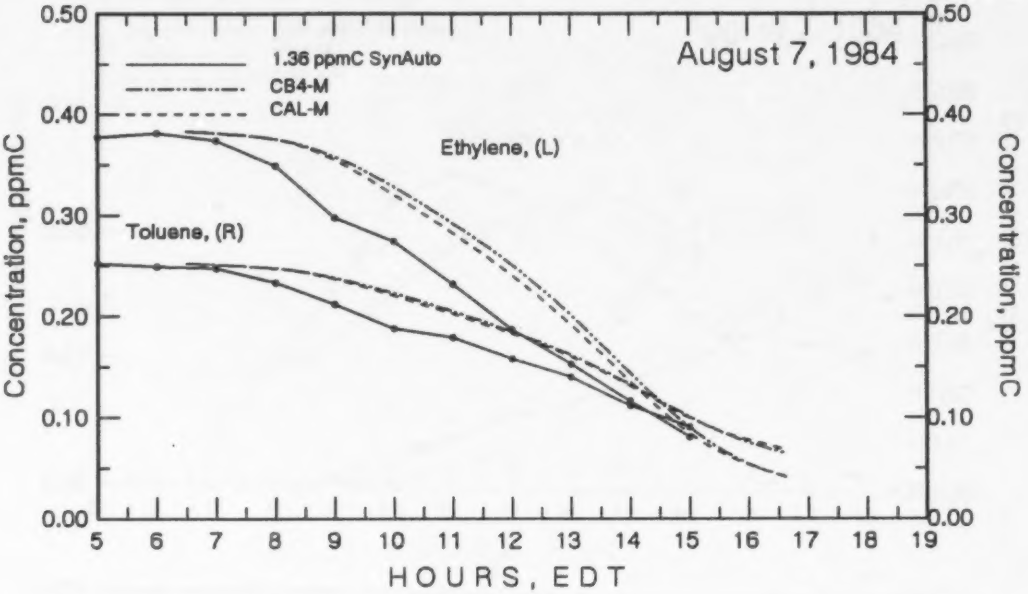


Figure A23. CB4-M and CAL-M Predictions.

-M



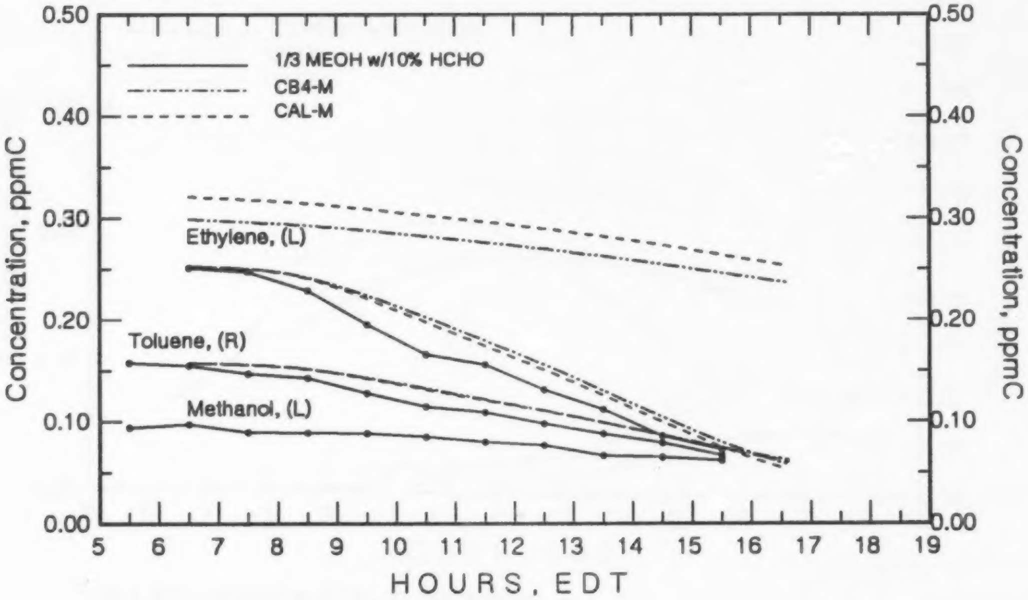
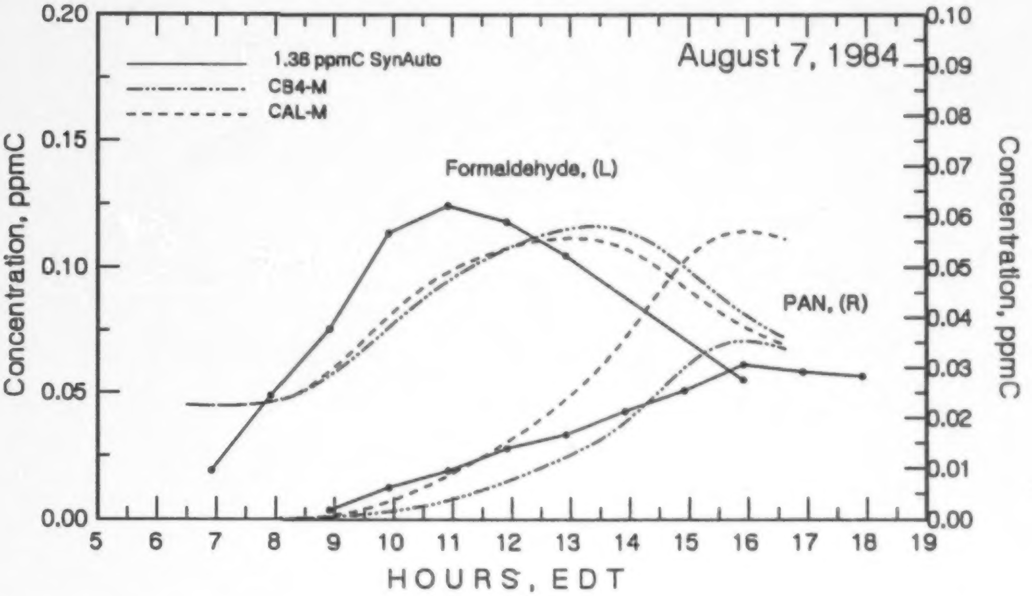


Figure A24. CB4-M and CAL-M Predictions.



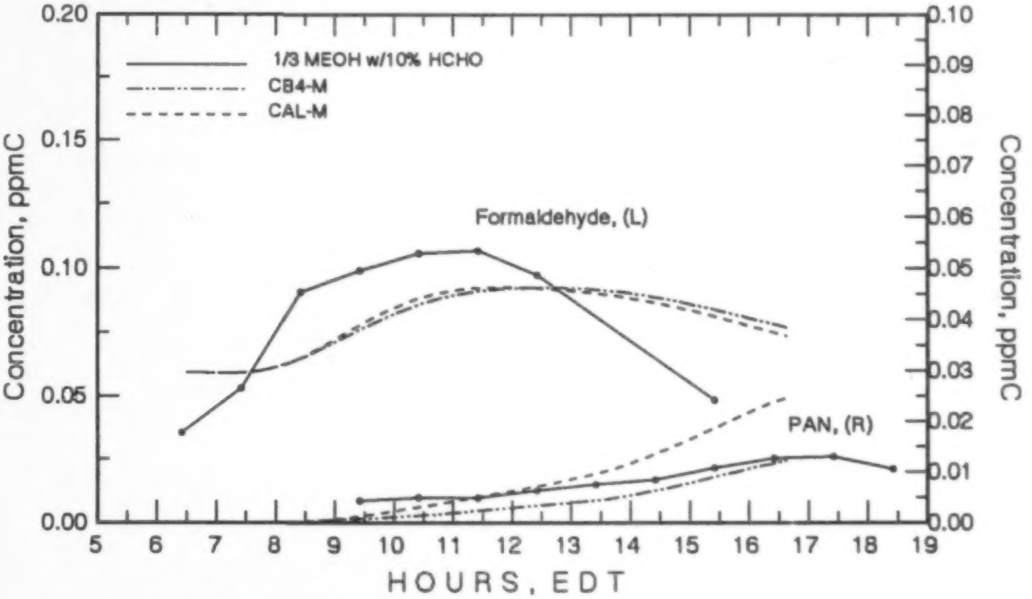


Figure A25. CB4-M and CAL-M Predictions.

August 8, 1984: 1/3 Methanol Substitution w/20% HCHO

Top: 2.5 ppmC SynAuto, 0.8 ppm MEOH, 0.2 ppm HCHO
Bottom: 3.7 ppmC SynAuto

Chamber Observations:

The temperature (Fig. A26) is below the dewpoint; thus, the timing of the model predictions can be expected to be late. The methanol substitution had no effect on the timing or concentration of ozone.

CB4 and CAL Predictions:

As expected, the predicted NO_x crossover points (Fig. A27) are late compared to the observed crossover points.

Given the timing delay, the hydrocarbon decay (Fig. A28) and ozone production (Fig. A27) profiles predicted by CB4 and CAL agree well with the profiles observed on both sides of the chamber.

The formaldehyde concentration profiles (Fig. A29) are predicted well by both mechanisms for both sides of the chamber. CAL over predicts the PAN concentrations on both sides of the chamber with P/O ratios equal to 1.4. CB4 also over predicts the PAN concentrations on the substitution side (top), but agrees well with the observed concentrations on the control side (bottom).

Addition of Methyl Nitrite:

Explicitly accounting for the presence of methyl nitrite (Figs. A30-2) shifts the predicted formaldehyde profile to the left closer to the observed concentration profile. Note that an error was made in the initial condition file for this experiment. Except for the concentrations of methyl nitirite and methanol the concentrations should be the same as those in the previous runs. This error is not expected to change the result.

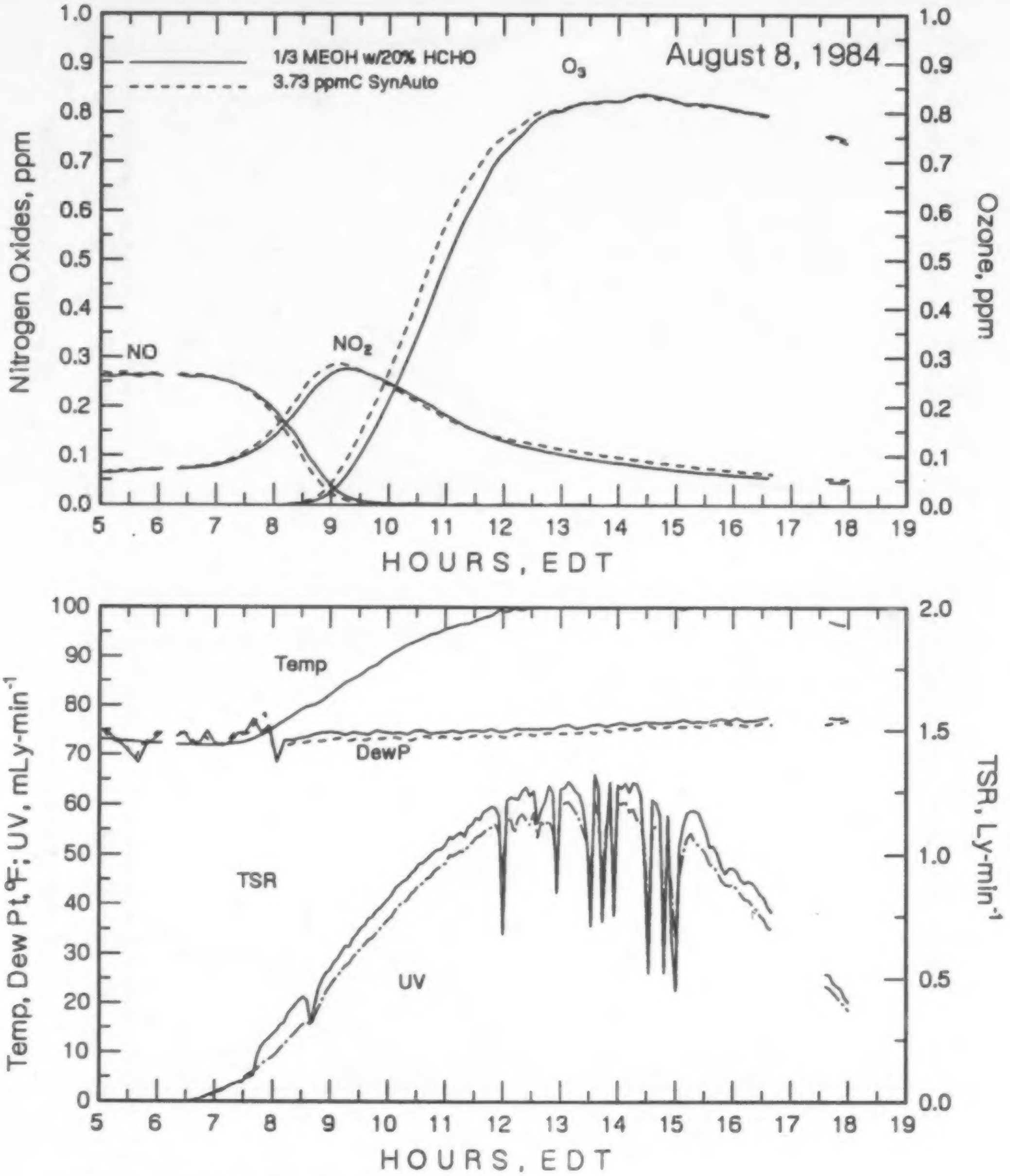


Figure A26. Chamber Observations.

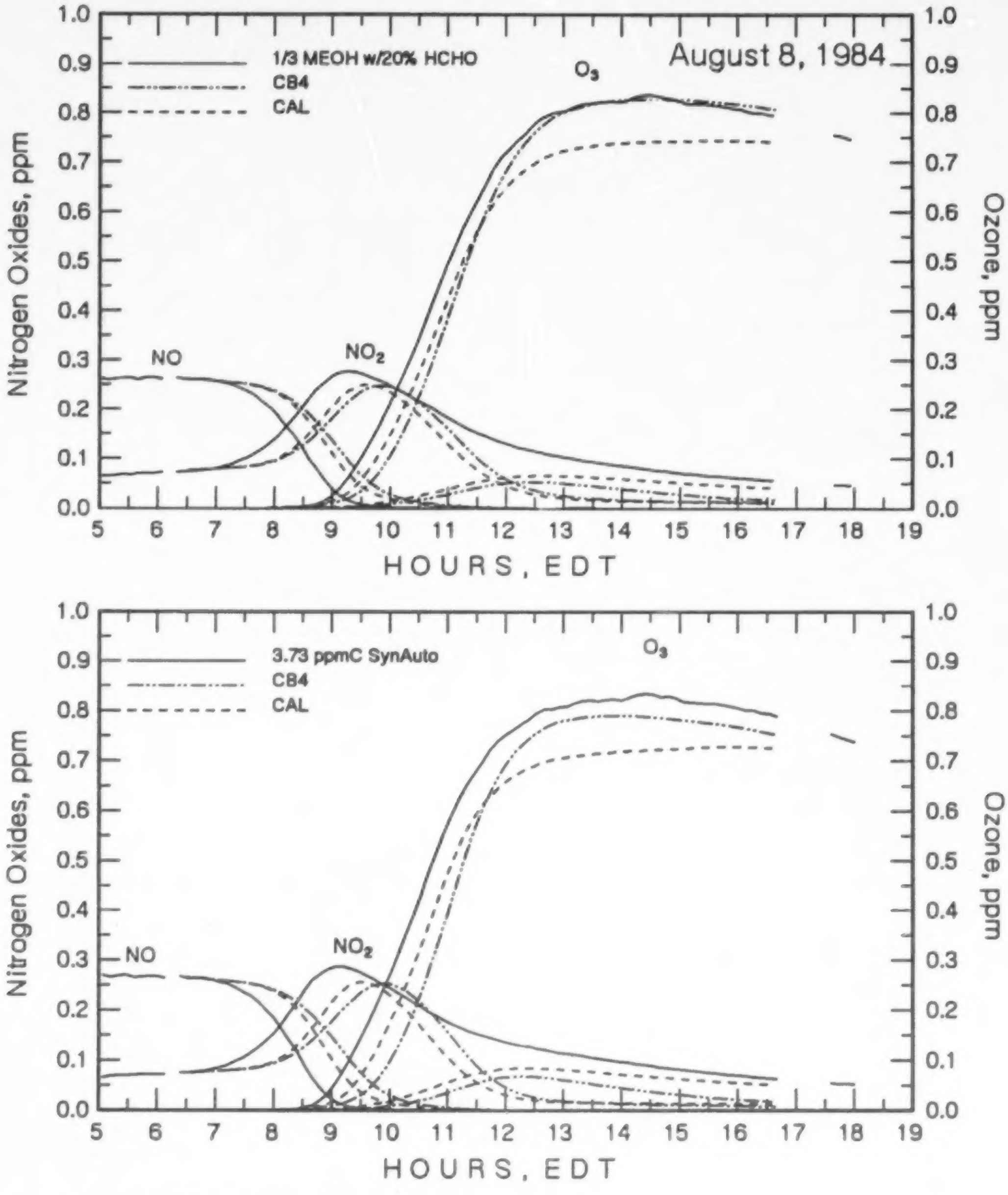


Figure A27. CB4 and CAL Predictions.

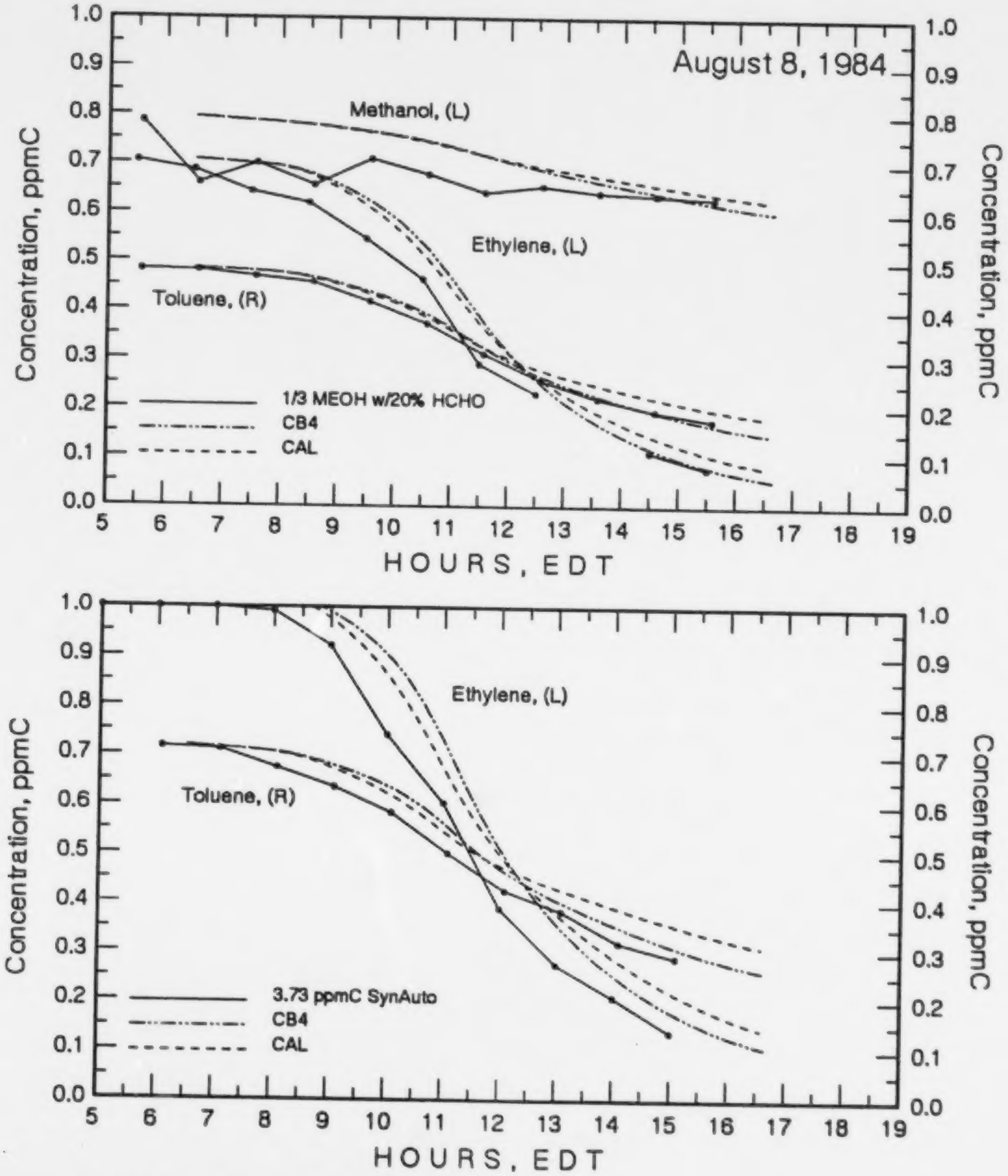


Figure A28. CB4 and CAL Predictions.

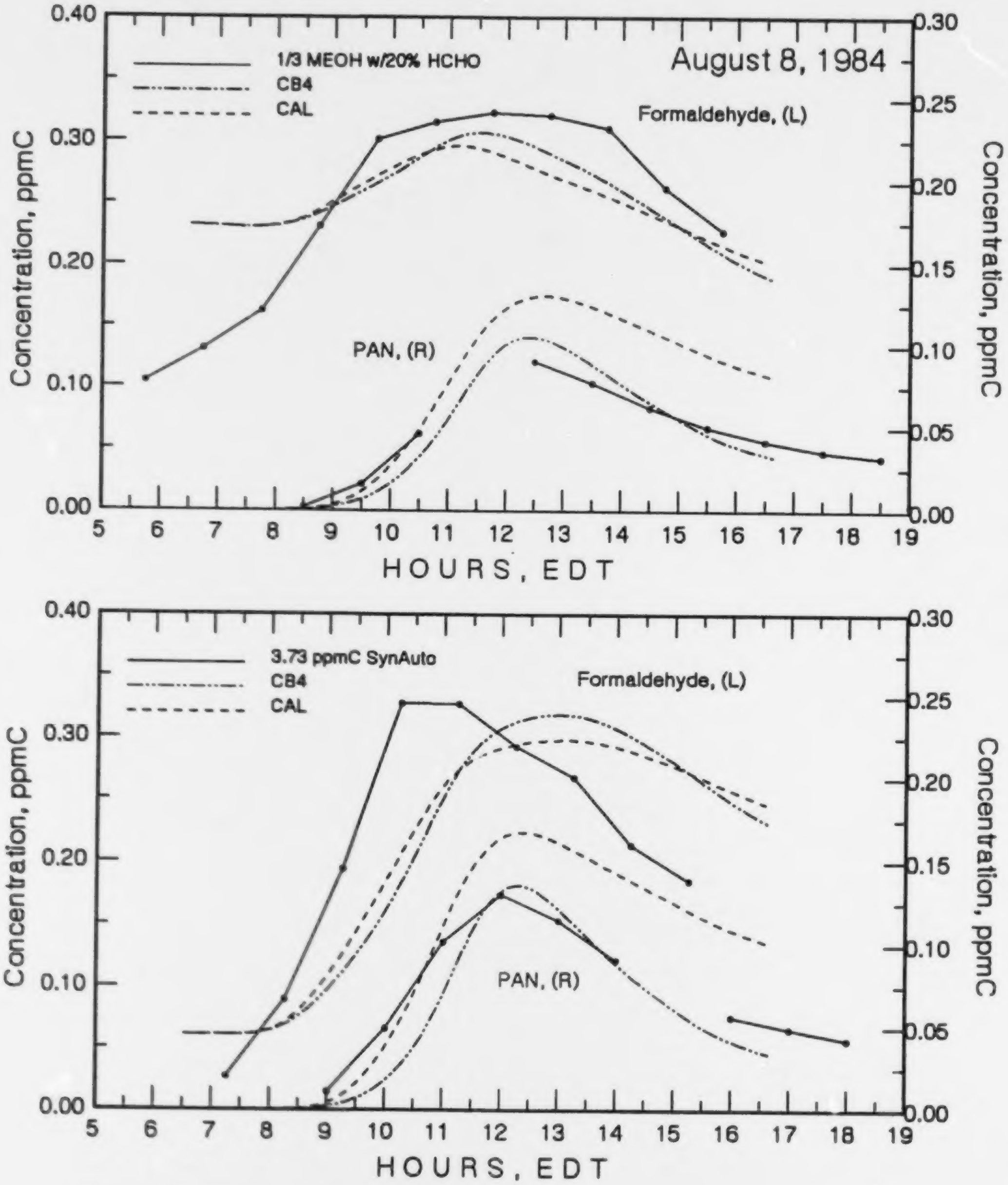
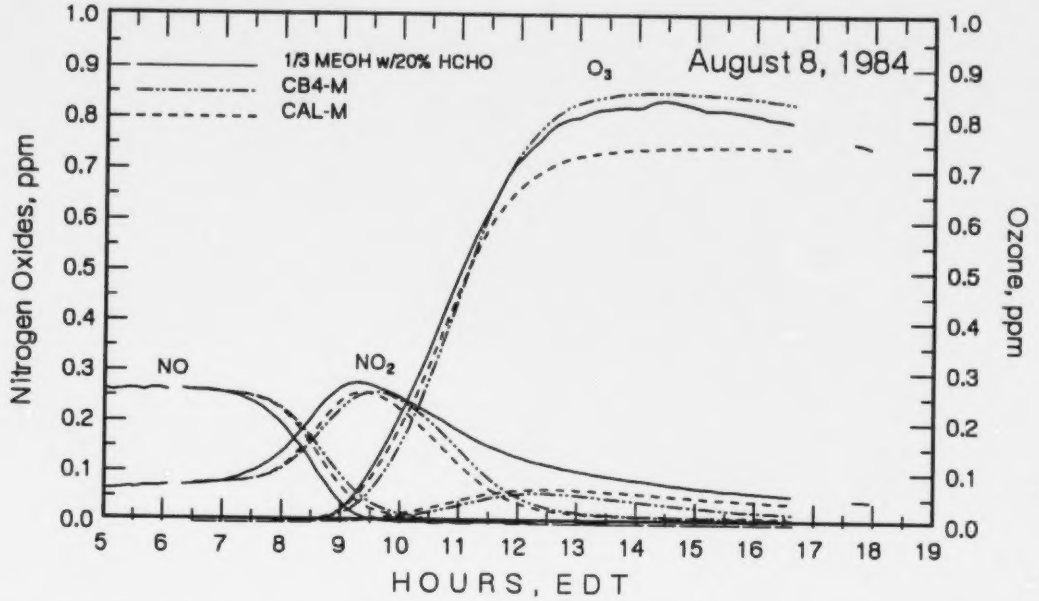


Figure A29. CB4 and CAL Predictions.



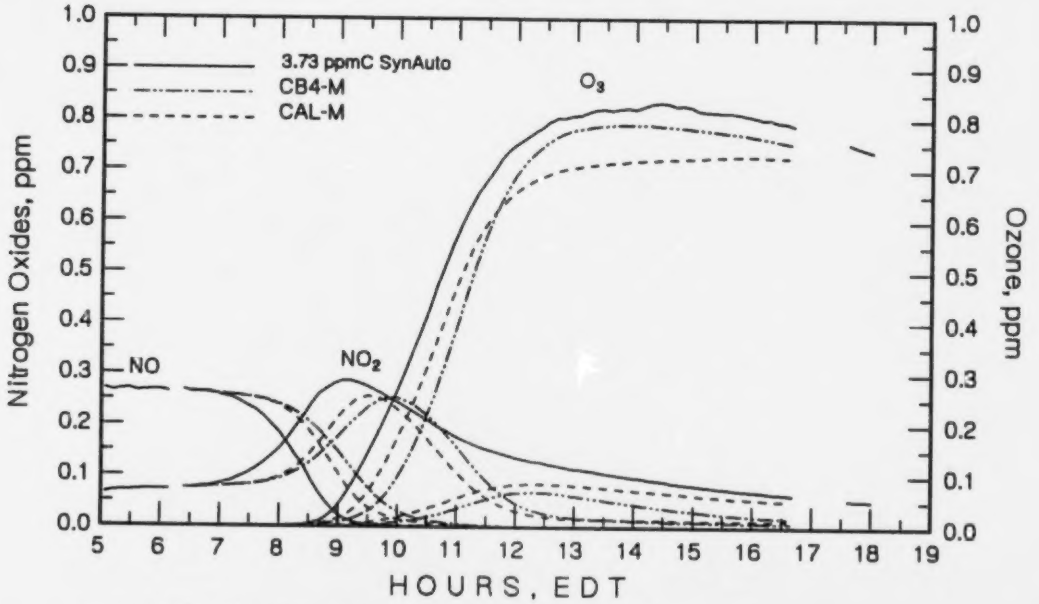
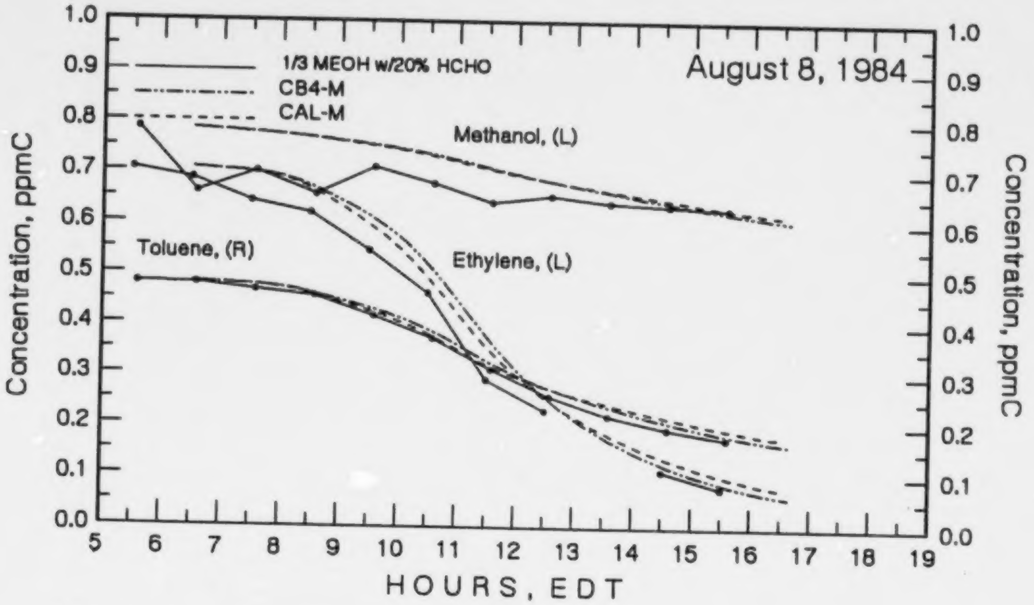


Figure A30. CB4-M and CAL-M Predictions.



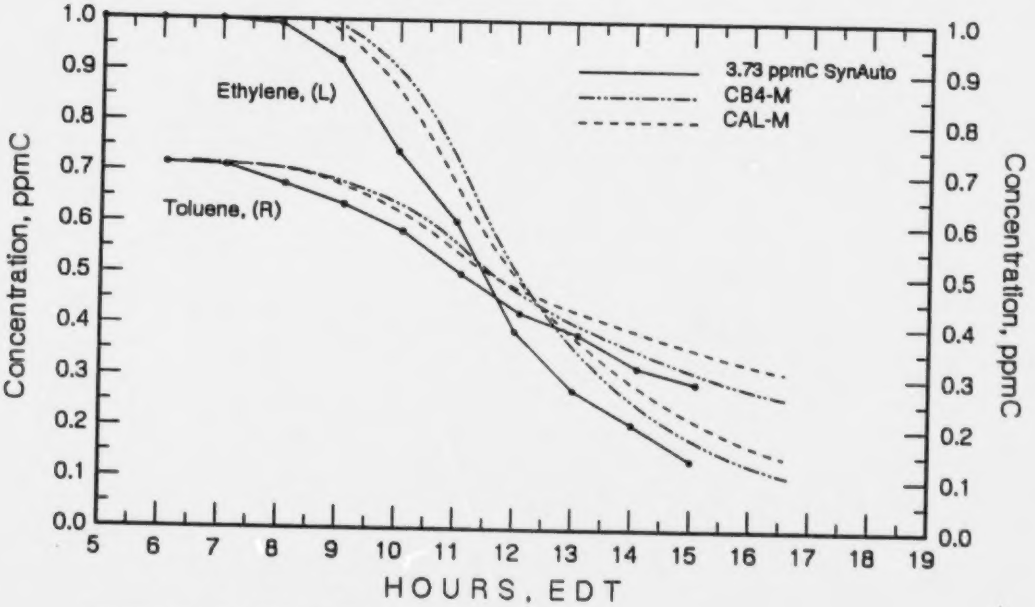


Figure A31. CB4-M and CAL-M Predictions.

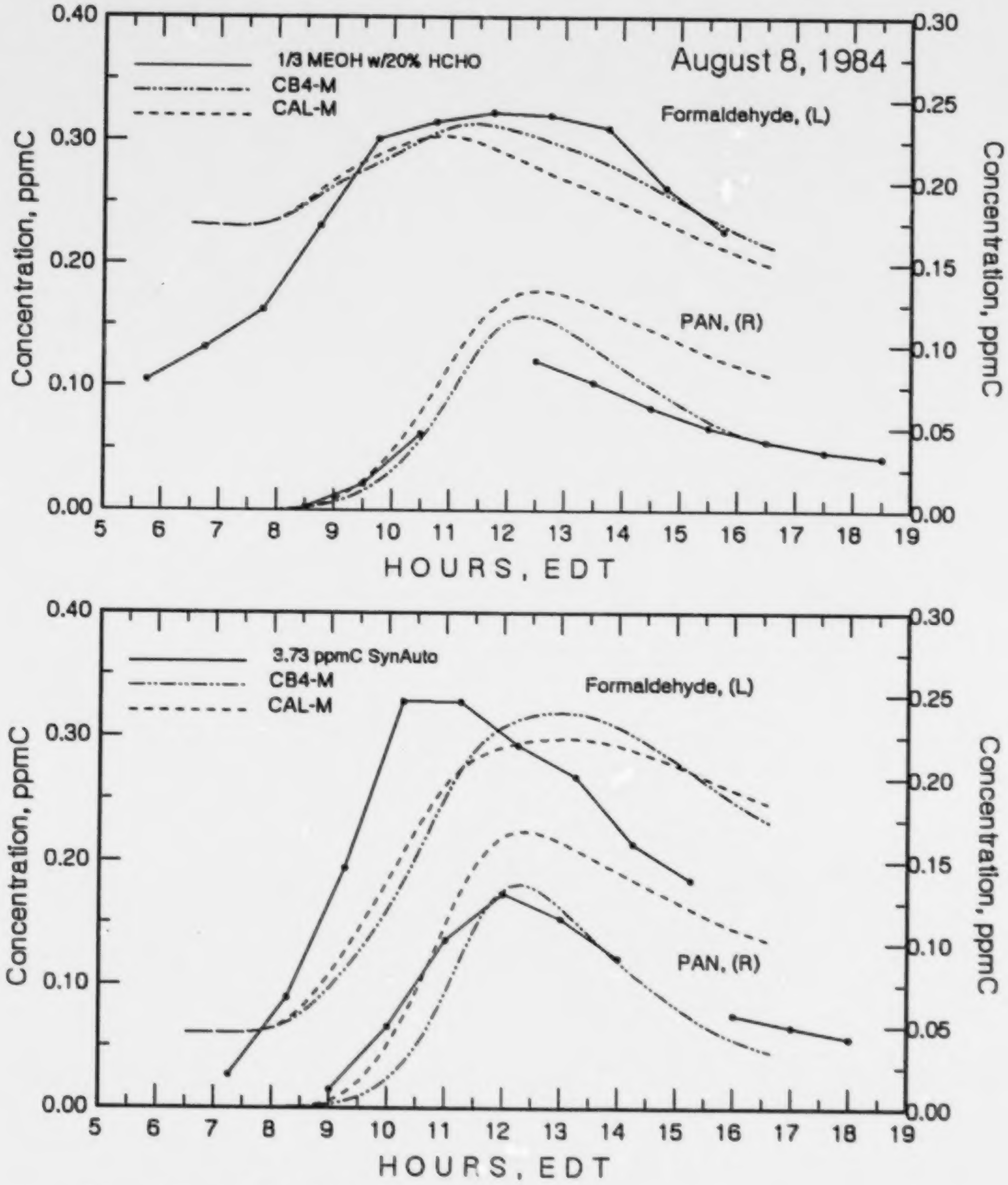


Figure A32. CB4-M and CAL-M Predictions.

August 9, 1984: 1/3 Methanol Substitution w/20% HCHO

Top: 1.30 ppmC SynAuto
Bottom: 0.87 ppmC SynAuto, 0.26 ppm MEOH, 0.06 ppm HCHO

Chamber Observations:

The temperature (Fig. A33) is below the dewpoint, and therefore, one expects the model predictions to be late compared to the observed data. The methanol substitution resulted in a reduction in the peak ozone concentration from 0.52 ppm to 0.32 ppm.

CB4 and CAL Predictions:

As expected, the predicted NO_x crossover points (Fig. A34) are late compared to the observed crossover points on both sides of the chamber.

The hydrocarbon decay profiles (Fig. A35) predicted by CB4 and CAL are late but have the correct shape, including the methanol decay profile on the substitution side (bottom).

Considering the timing problem, the ozone concentration profiles (Fig. A34) predicted by CB4 and CAL agree with the observed profiles on both sides of the chamber.

CB4 and CAL under predict the formaldehyde concentrations (Fig. A36) on both sides of the chamber with an approxiamate P/O ratio of 0.6. The PAN concentrations predicted by CB4 agree well with the observed concentrations given the timing problem. CAL, however, over predicts PAN concentrations on both sides of the chamber with P/O ratios equal to approxiamately 1.7.

Addition of Methyl Nitrite:

Explicitly accounting for the presence of methyl nitrite (Figs. A37-9), shifts the predicted formaldehyde profile to the left but does not increase the predicted peak concentration.

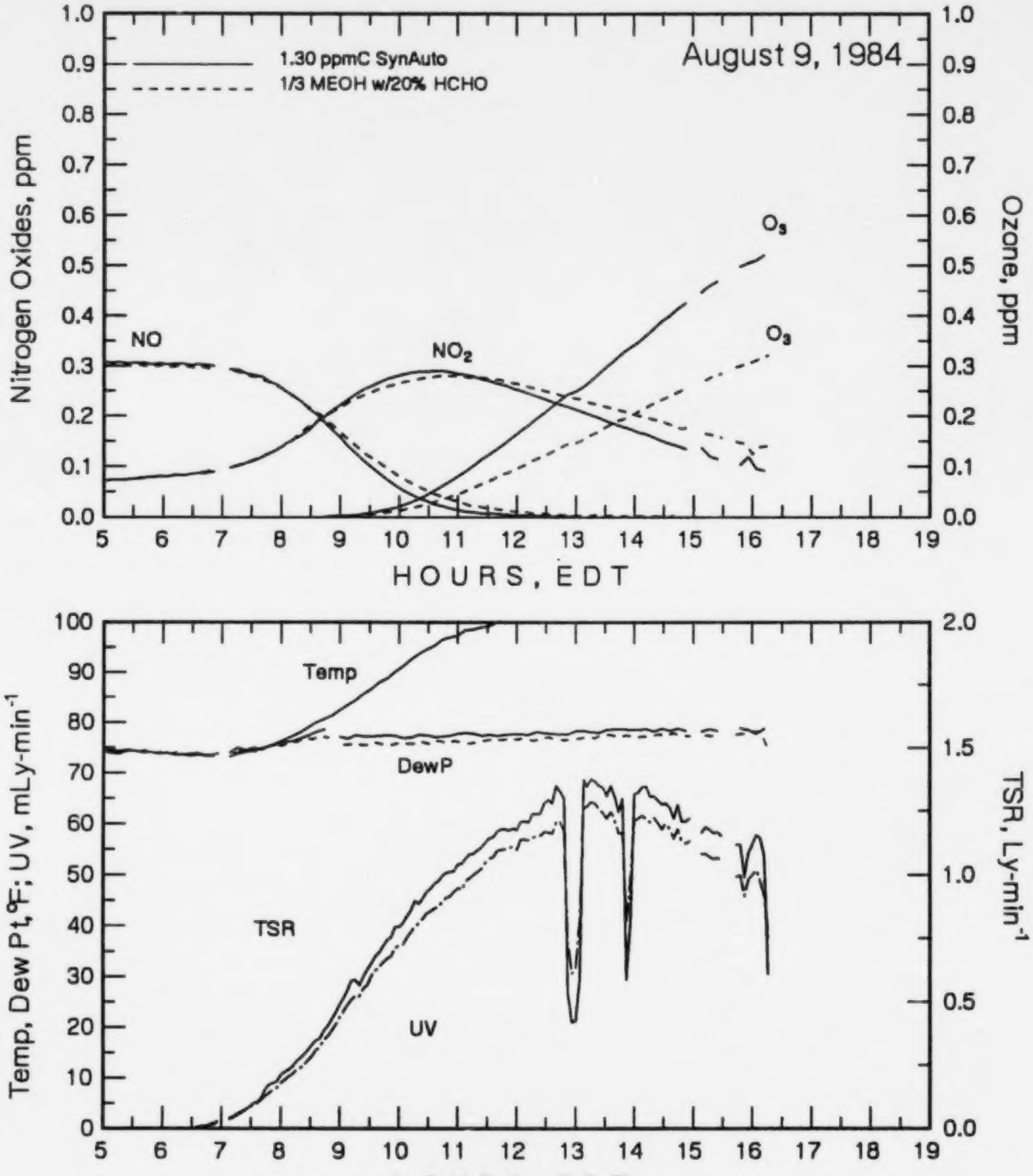
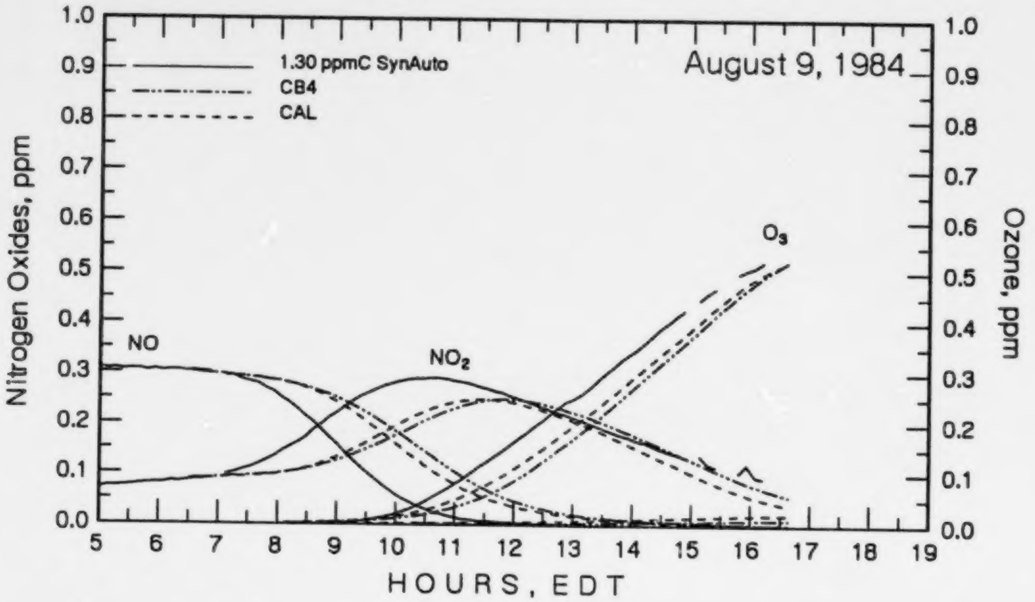


Figure A33. Chamber Observations.



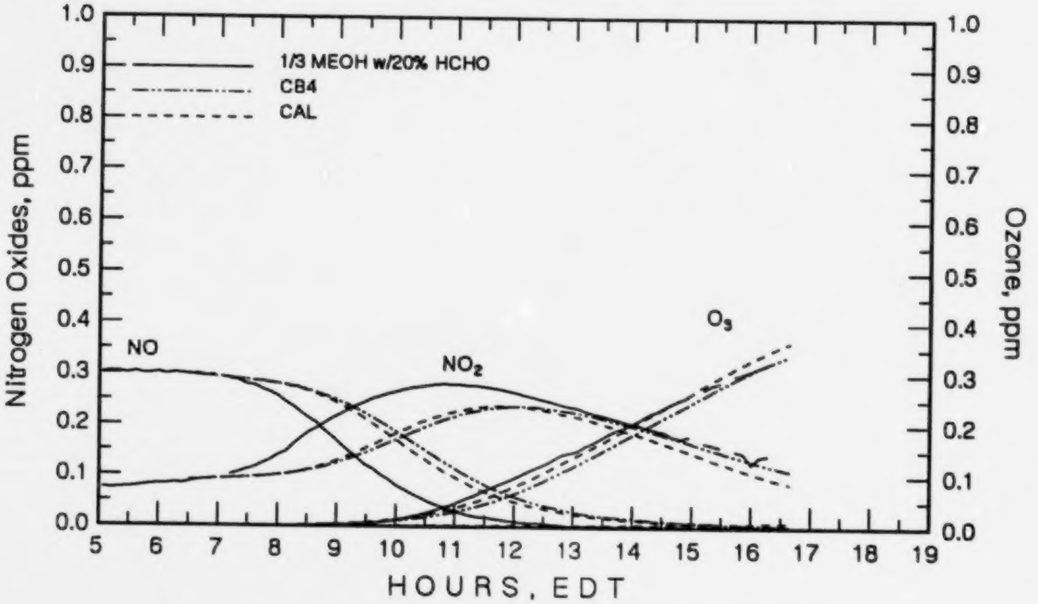


Figure A34. CB4 and CAL Predictions.

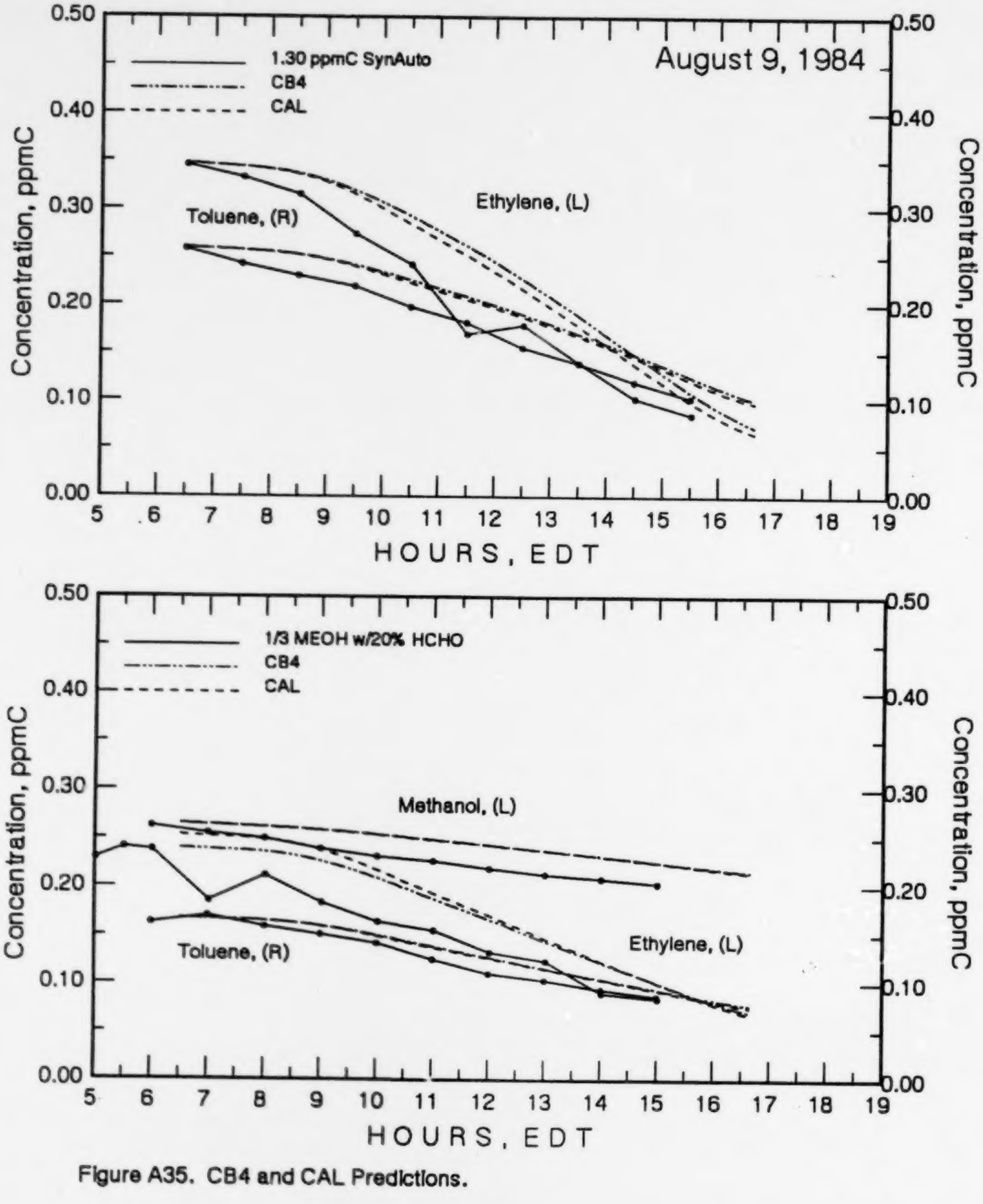
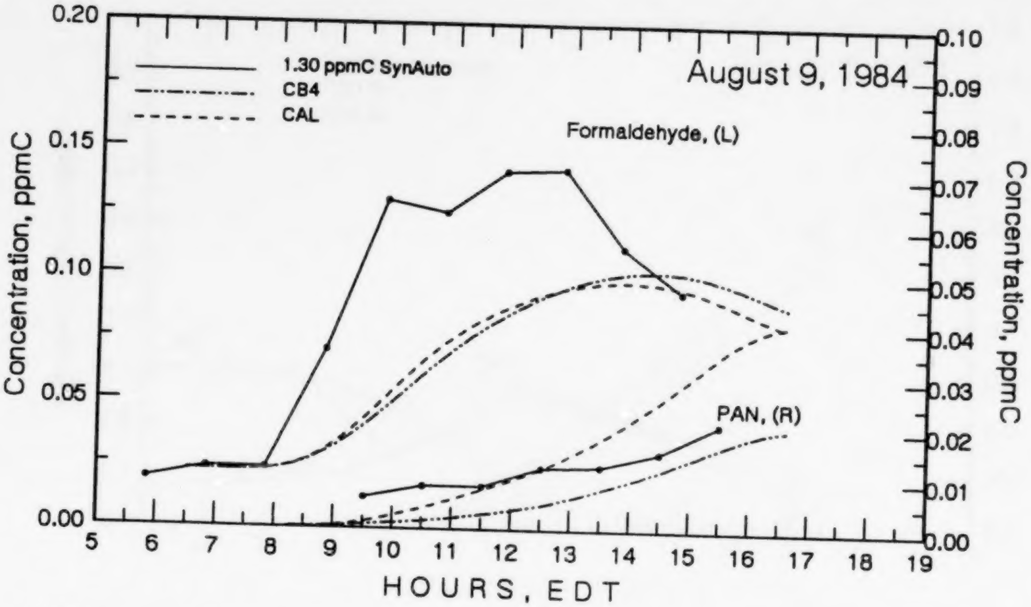


Figure A35. CB4 and CAL Predictions.



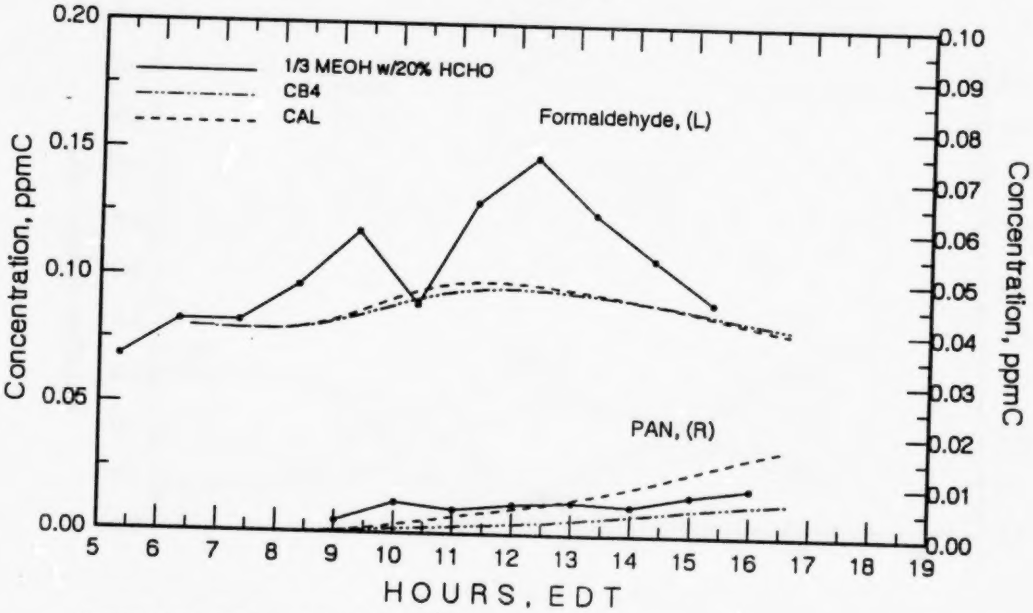


Figure A36. CB4 and CAL Predictions.

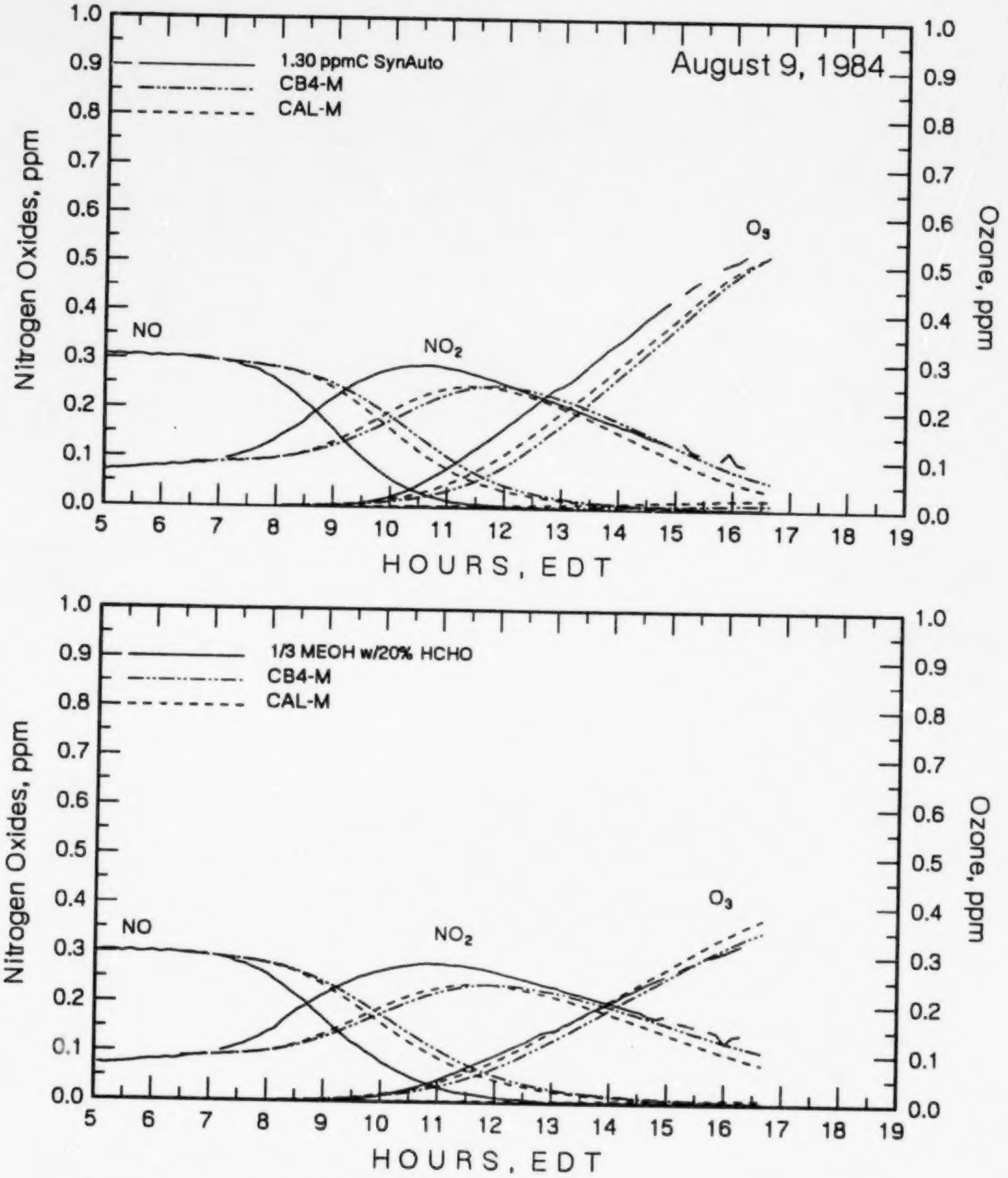


Figure A37. CB4-M and CAL-M Predictions.

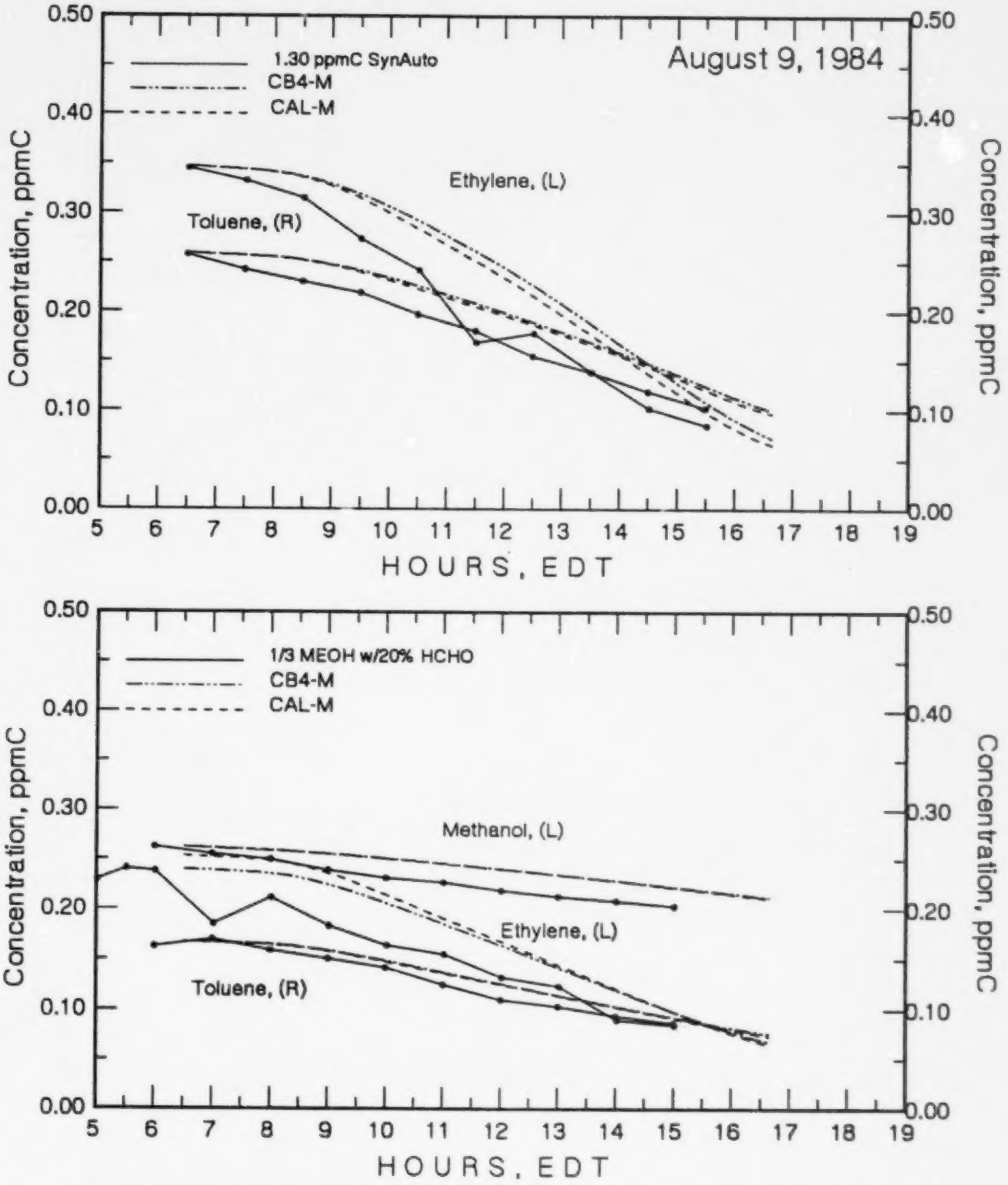


Figure A38. CB4-M and CAL-M Predictions.

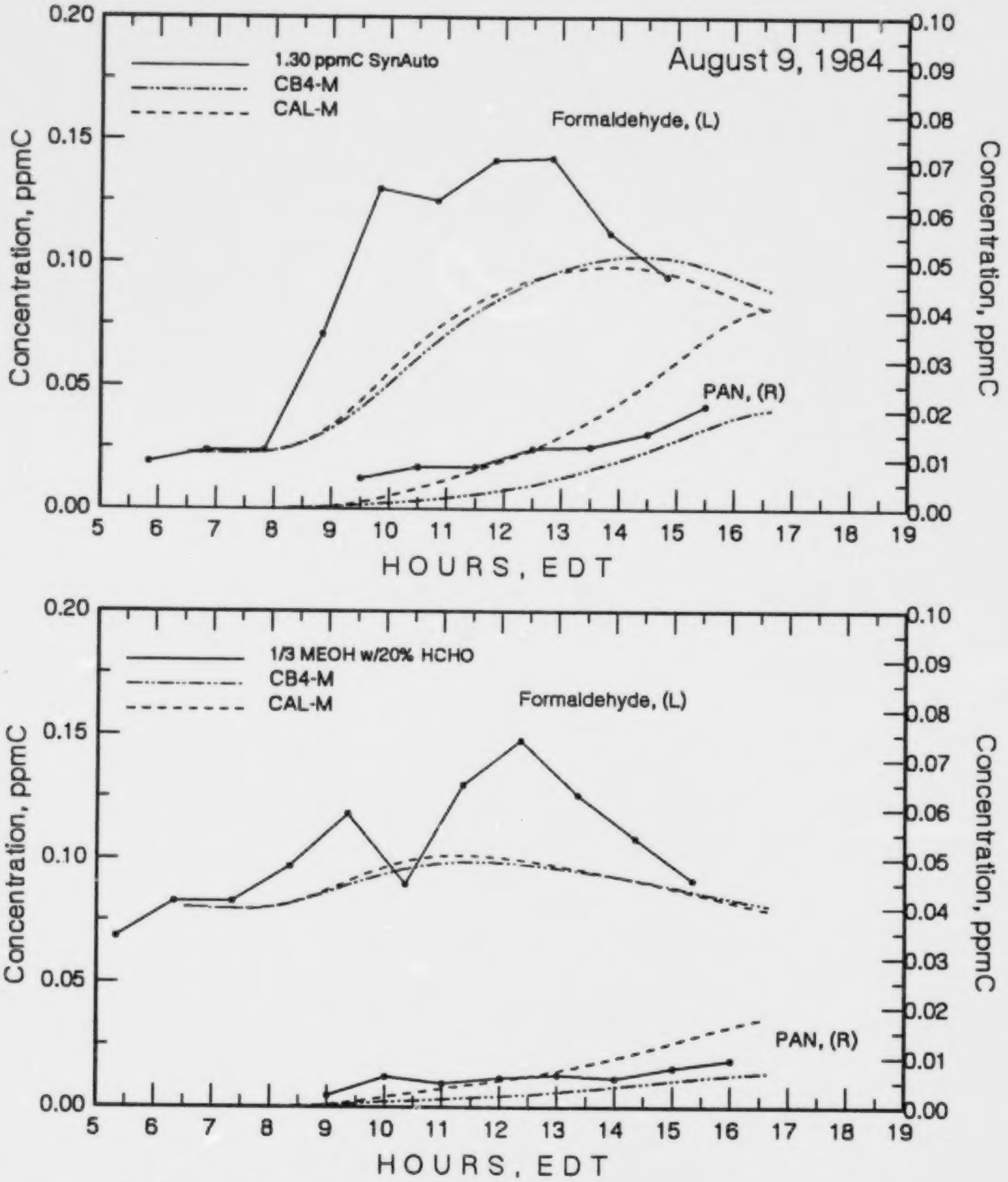


Figure A39. CB4-M and CAL-M Predictions.

August 22, 1984: 1/3 Methanol Substitution w/20% HCHO

Top: 3.2 ppmC SynUrban
Bottom: 2.2 ppmC SynUrban, 0.9 ppm MEOH, 0.09 ppm HCHO

Chamber Observations:

In Figure A40, there is no change in the ozone concentrations produced due to the methanol substitution.

CB4 and CAL Predictions:

The NO_x crossover points (Fig. A41) predicted by CB4 and CAL are close to the observed crossover points on both sides of the chamber.

The hydrocarbon decay profiles (Fig. A42) predicted by CB4 and CAL agree with the observed profiles, except for methanol on the substitution side (bottom).

Both mechanisms over predict the ozone concentration profiles (Fig. A41) on both sides of the chamber with P/O ratios of 1.3 and 1.2 for CB4 and CAL, respectively.

In Figure A43, there is very little formaldehyde data to compare to the model predictions, but it does appear that both CB4 and CAL under predict the formaldehyde concentration profiles with P/O ratios of 0.7 and 0.8 for the control side (top) and the substitution side (bottom), respectively. There are no PAN concentration observations to compare to the model predictions.

CIT Predictions:

The NOx crossover points (Fig. A44) and the ethylene decay profiles (Fig. A45) are predicted correctly by both CIT mechanisms. The methanol decay profiles predicted by the CIT mechanisms are very close to the profiles predicted by CB4 and CAL, which suggests that the models all produced similar quantities of OH radicals.

CIT-1 is much too reactive and greatly over predicts the peak ozone concentrations (Fig. A44). CIT-2, however, tracks the ozone concentration profiles better than CB4 or CAL until the late afternoon. CIT-2 predicts that ozone production continues at a constant rate throughout the afternoon instead of slowing down as NO2 concentrations decrease, and consequently, it over predicts the final ozone concentrations on both sides of the chamber.

In Figure A46, CIT-1 again appears to be much too reactive. CIT-2, however, under predicts the formaldehyde concentrations on both sides of the chamber with P/O ratios of about 0.7. The PAN concentrations predicted by CIT-1 and CIT-2 are only 10 to 20% of the amount of PAN predicted by CB4 and CAL.

Addition of Methyl Nitrite:

The explicit representation of methyl nitrite (Figs. A47-9) causes more formaladhyde to be produced earlier and increases the predicted peak concentration of formaldehyde.

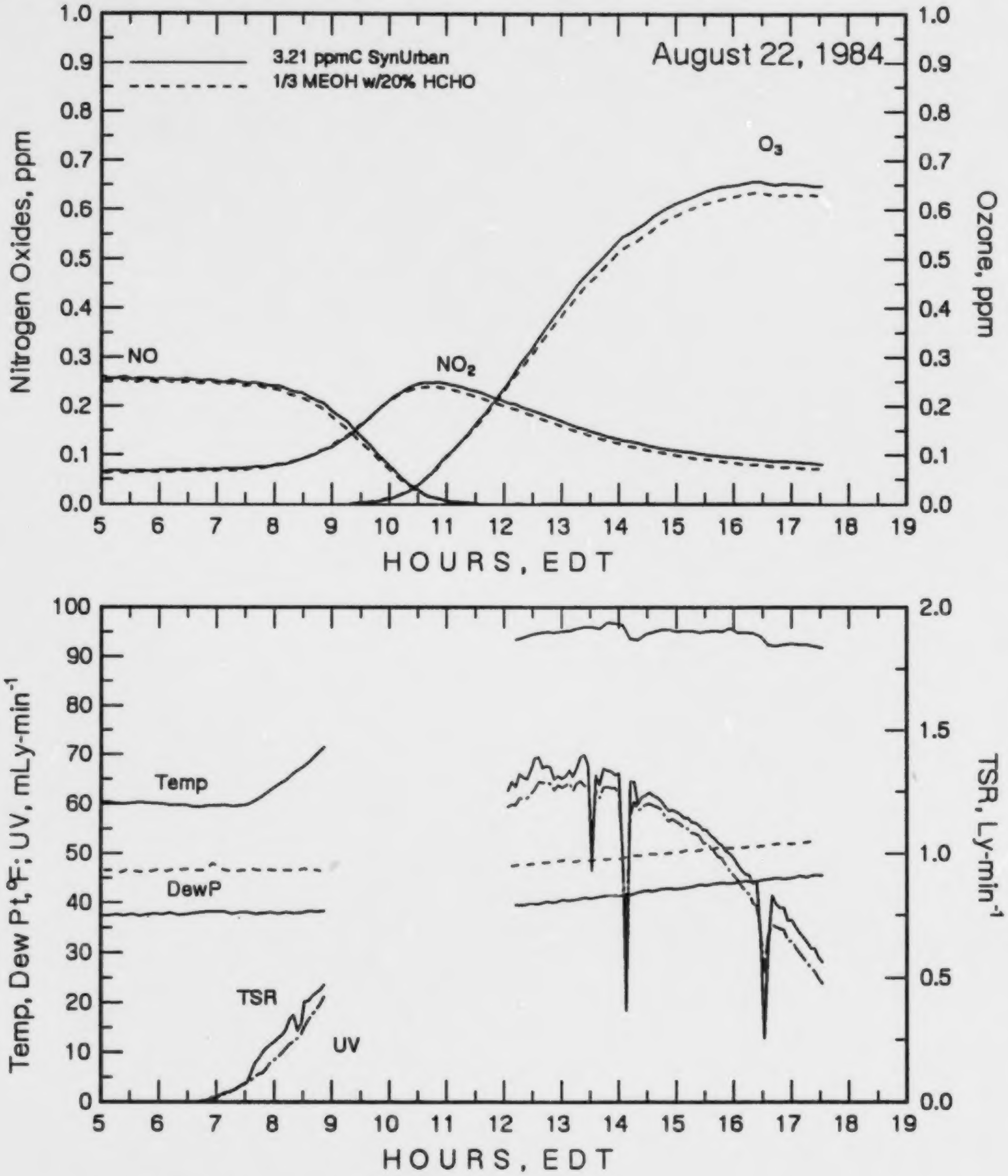
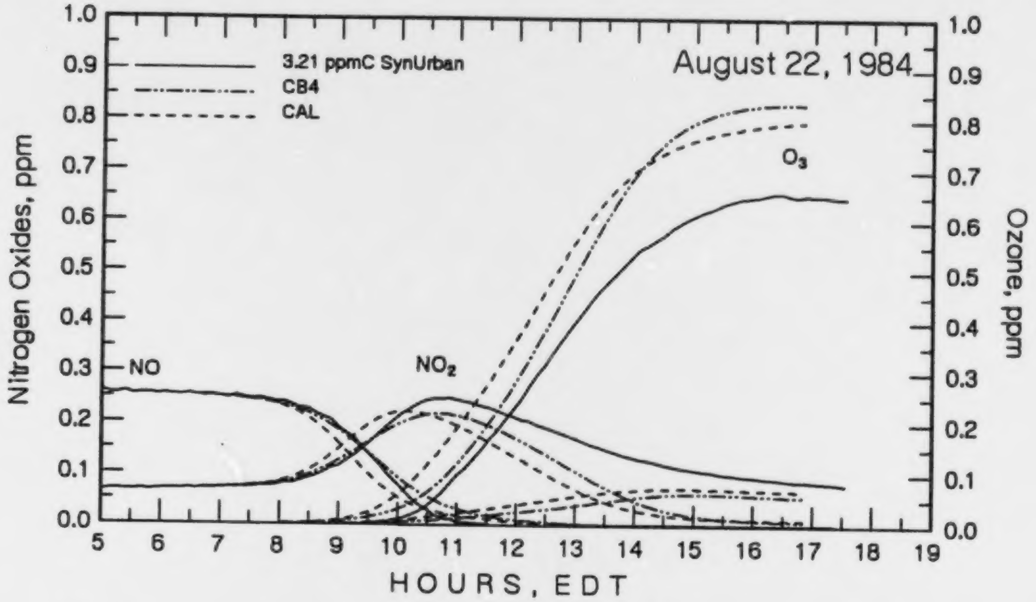


Figure A40. Chamber Observations.



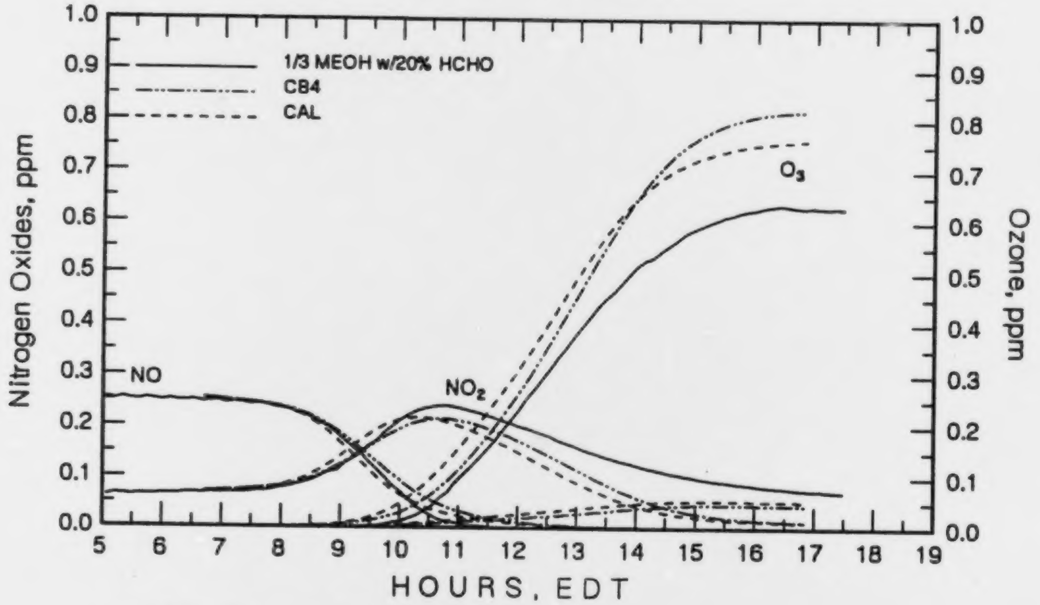


Figure A41. CB4 and CAL Predictions.

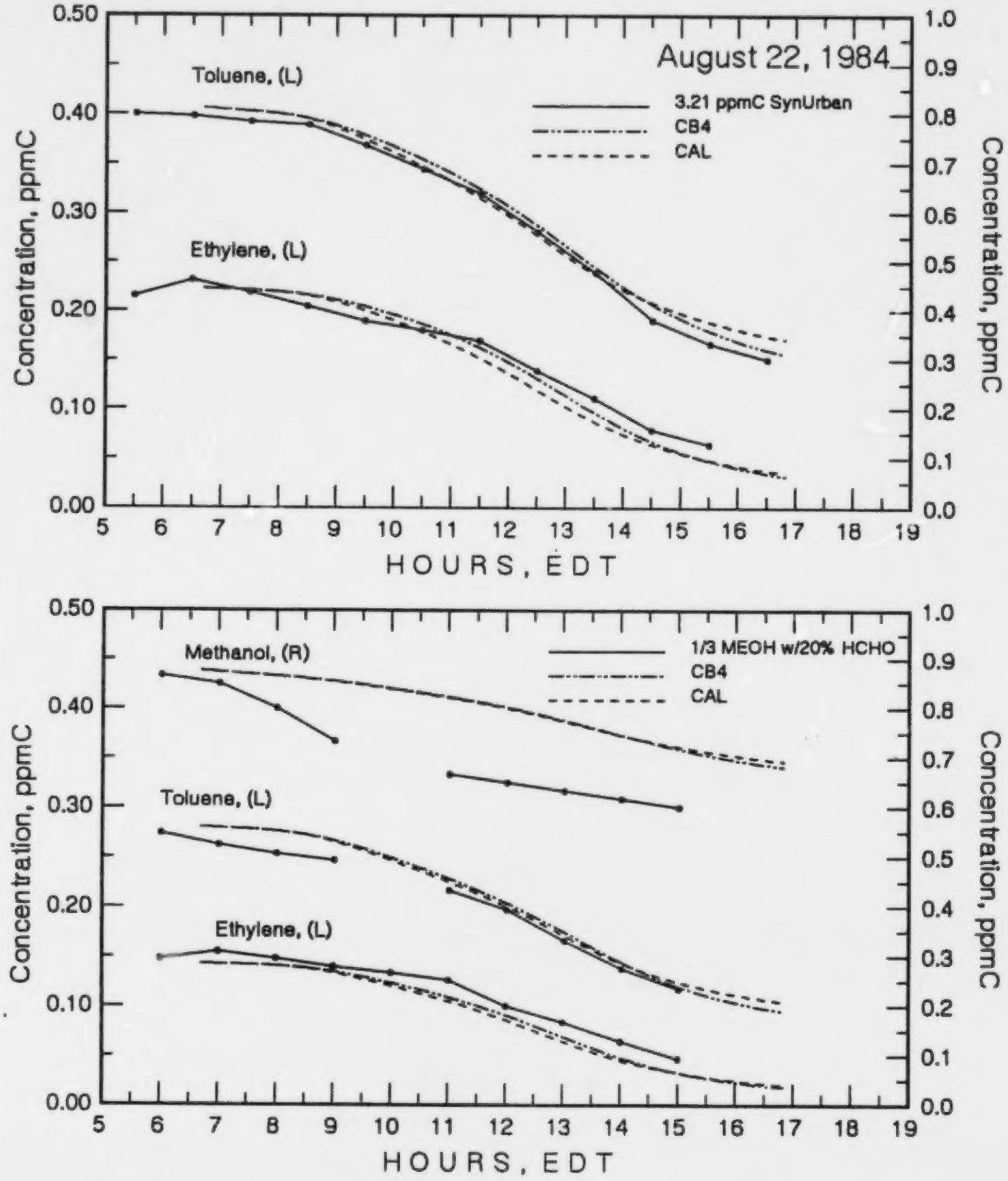


Figure A42. CB4 and CAL Predictions.

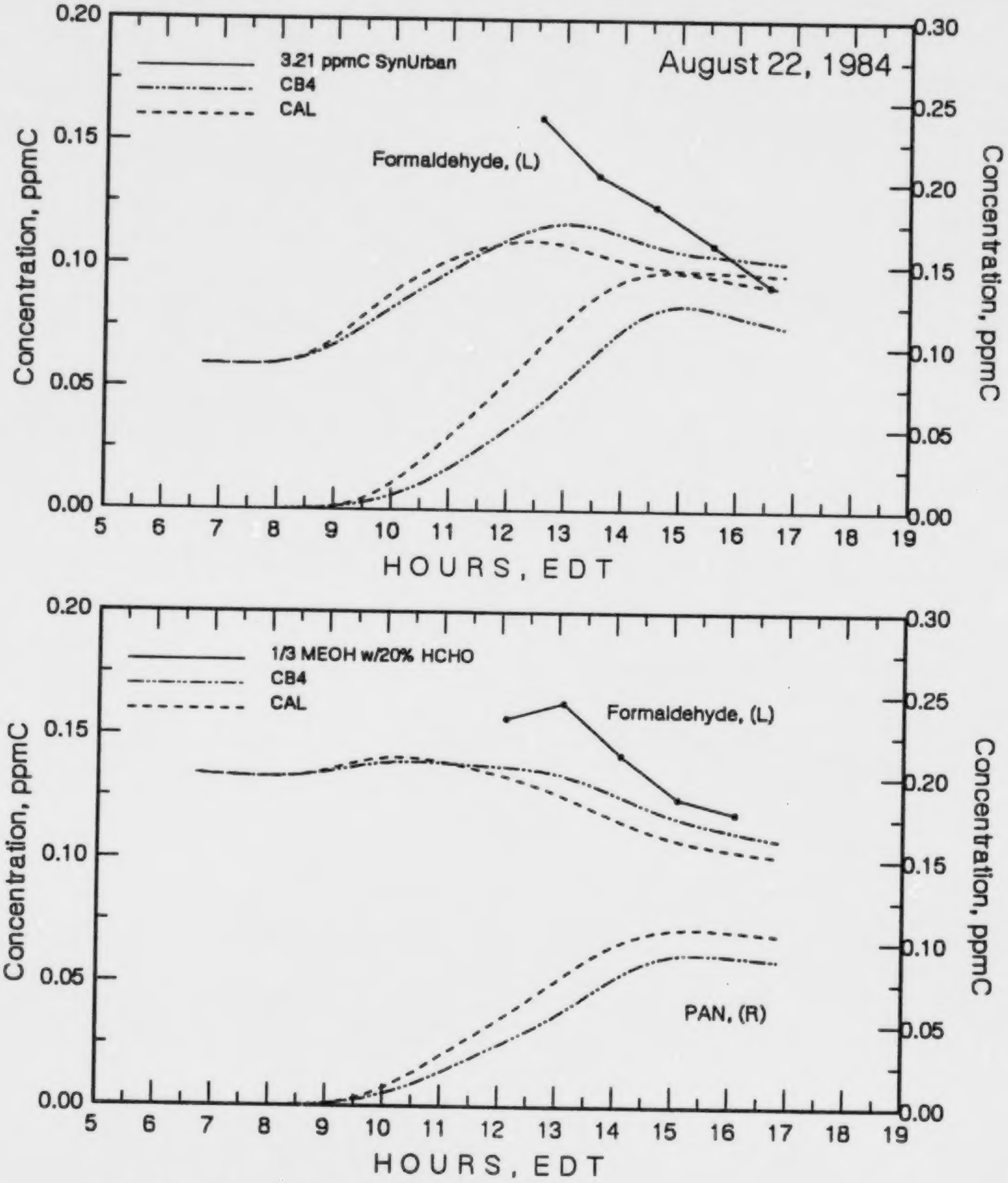
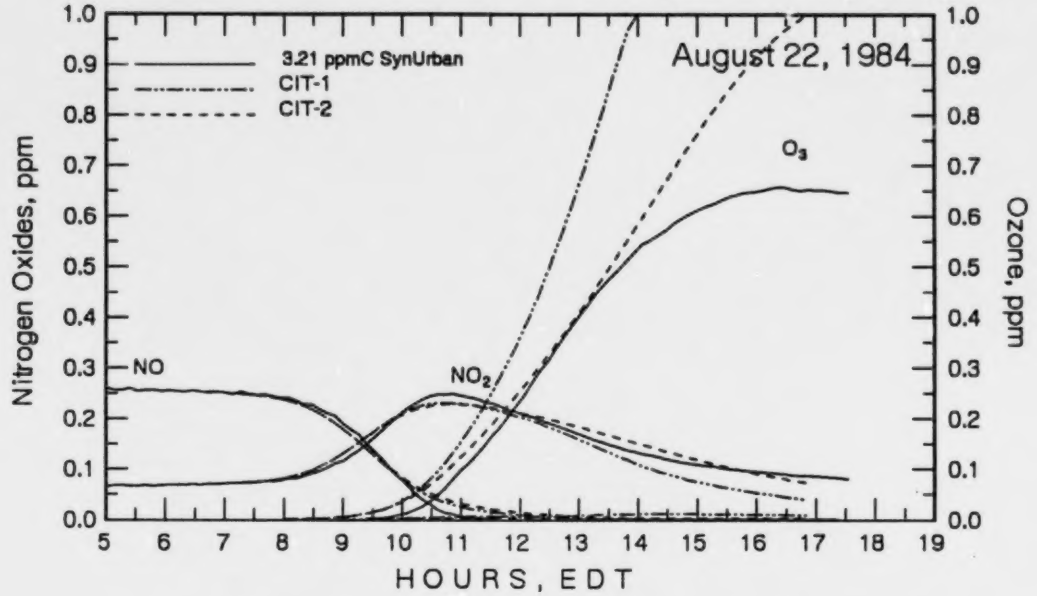


Figure A43. CB4 and CAL Predictions.



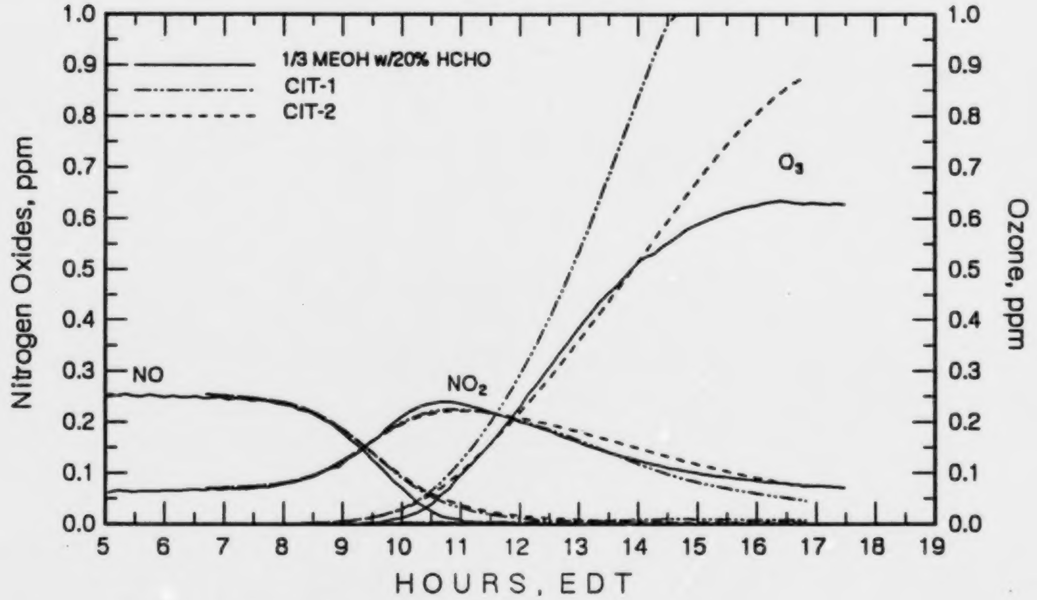


Figure A44. CIT Predictions.

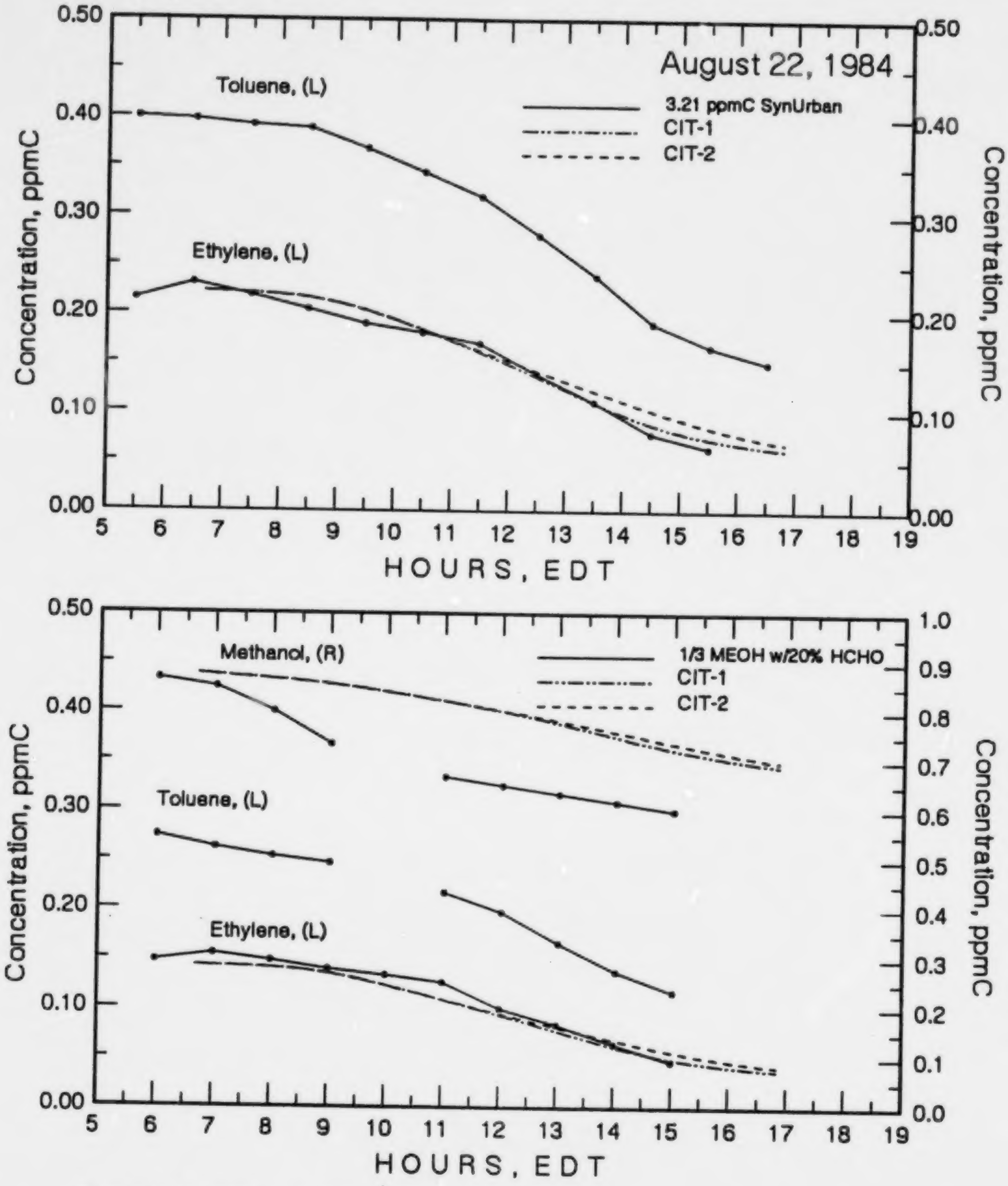


Figure A45. CIT Predictions.

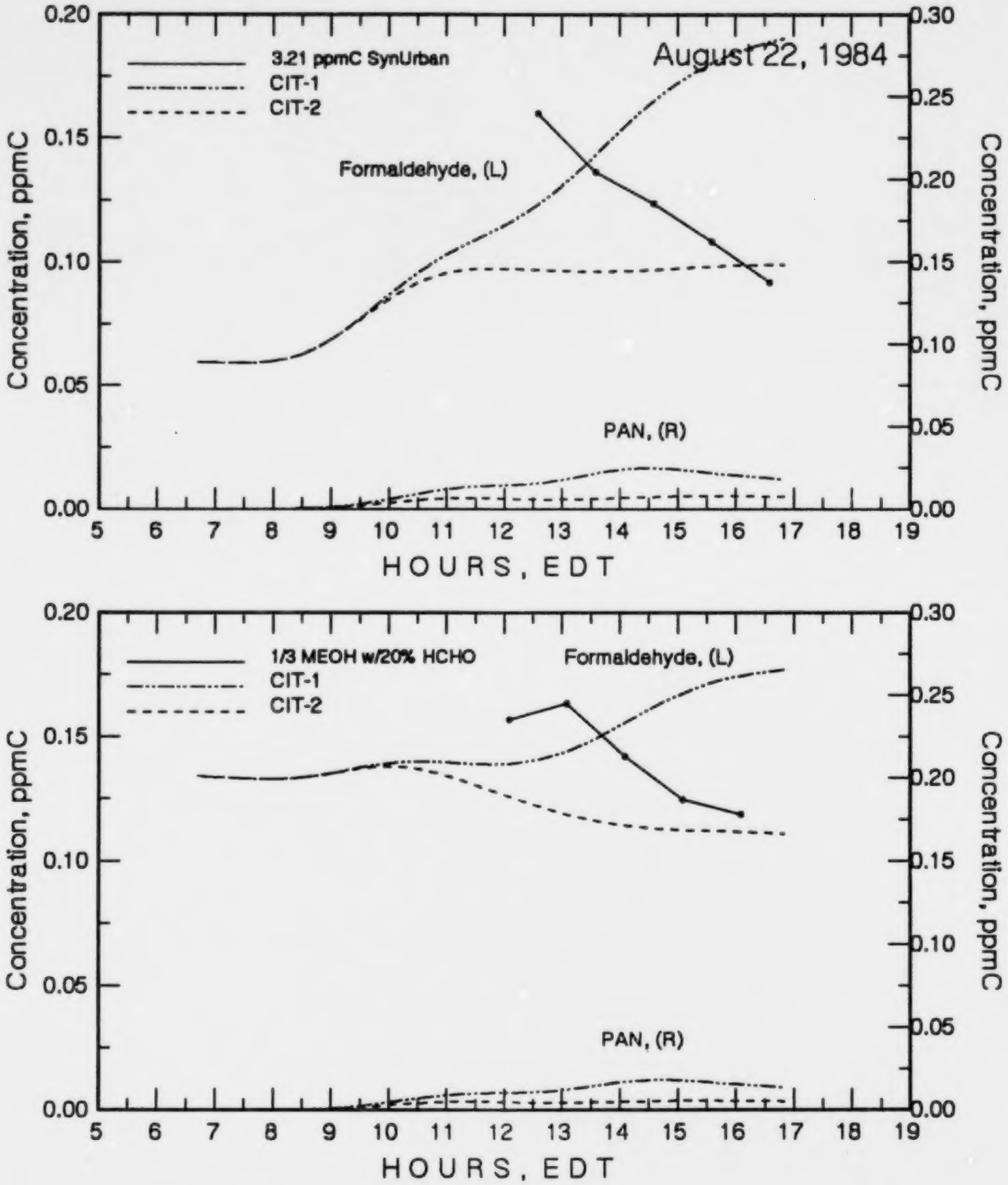


Figure A46. CIT Predictions.

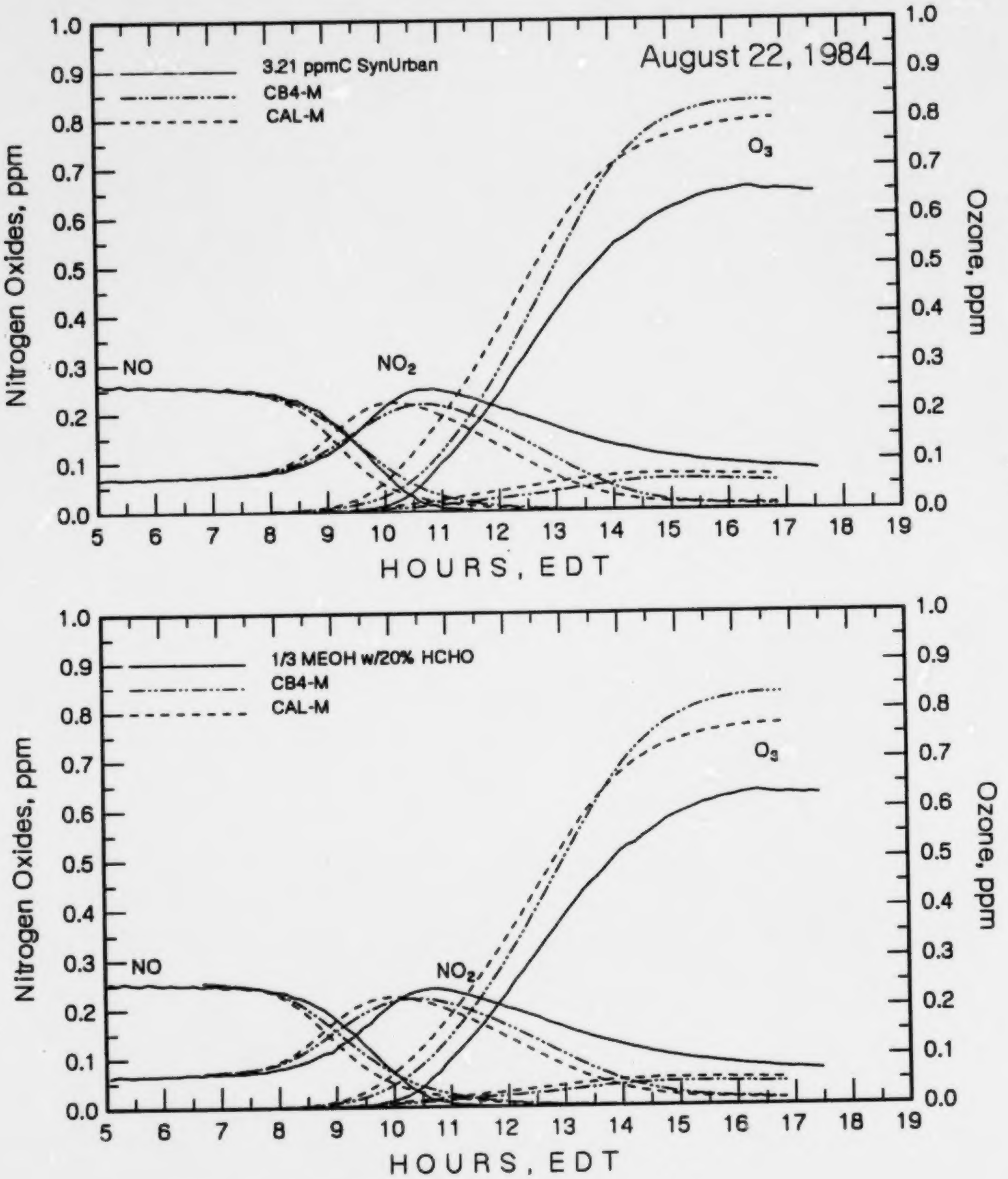
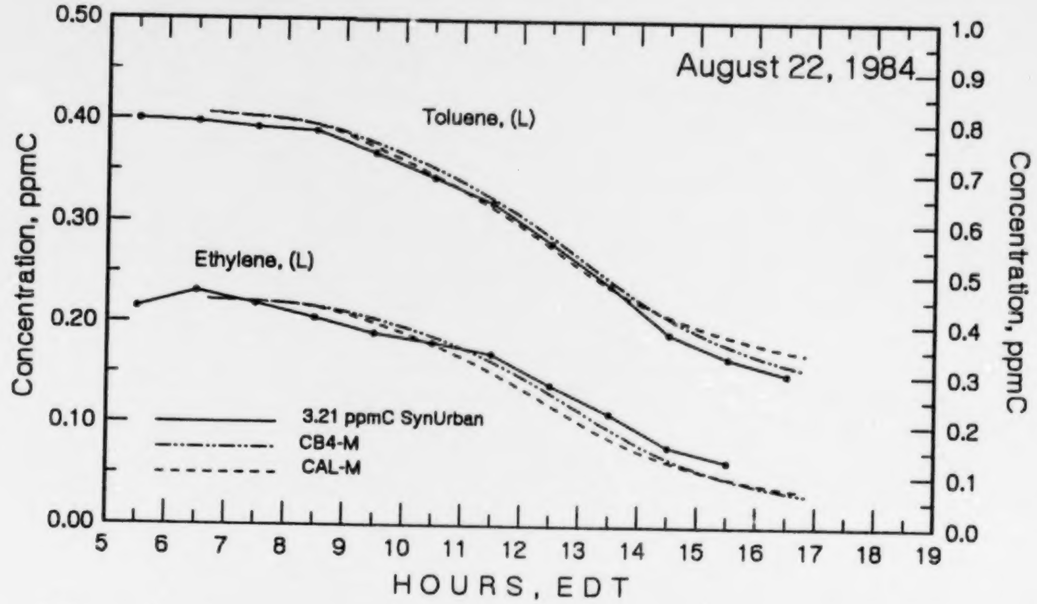


Figure A47. CB4-M and CAL-M Predictions.



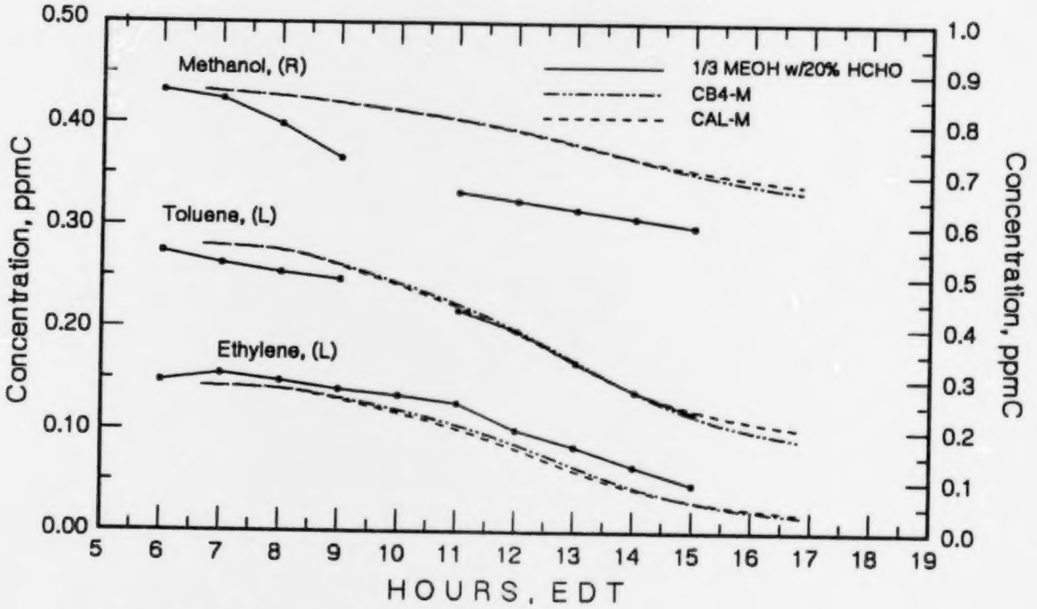
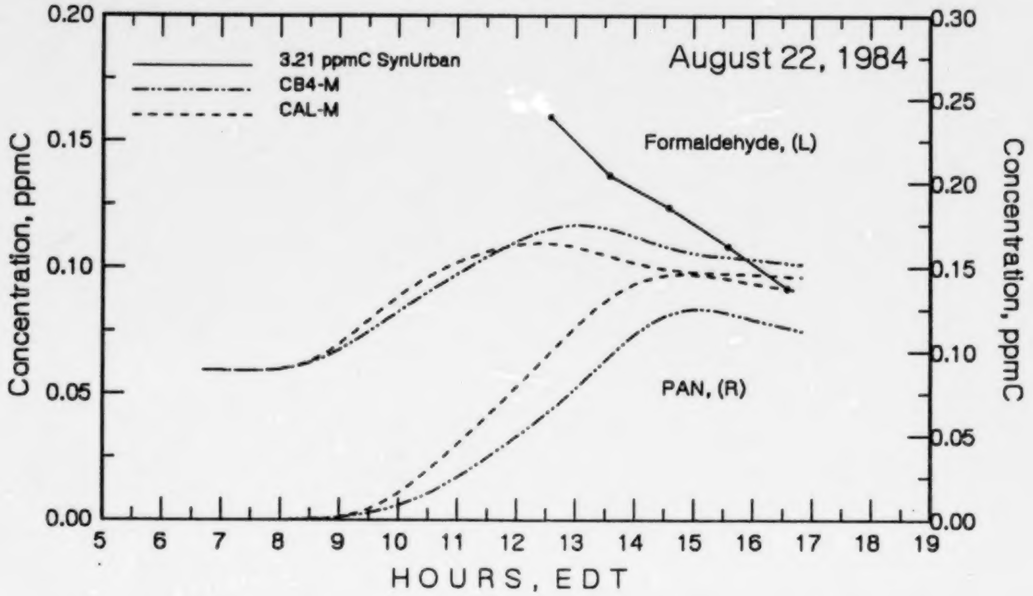


Figure A48. CB4-M and CAL-M Predictions.



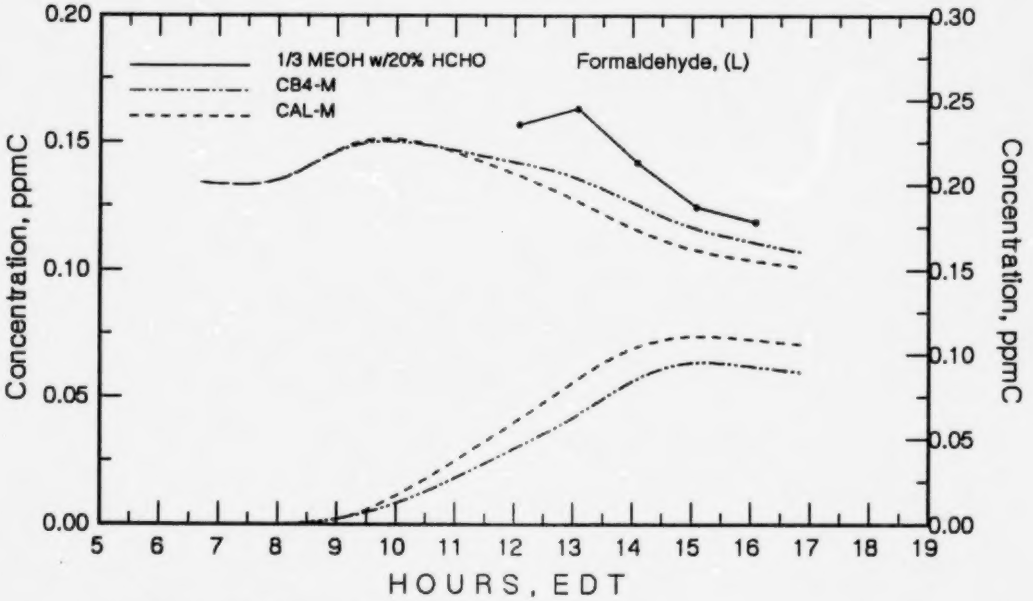


Figure A49. CB4-M and CAL-M Predictions.

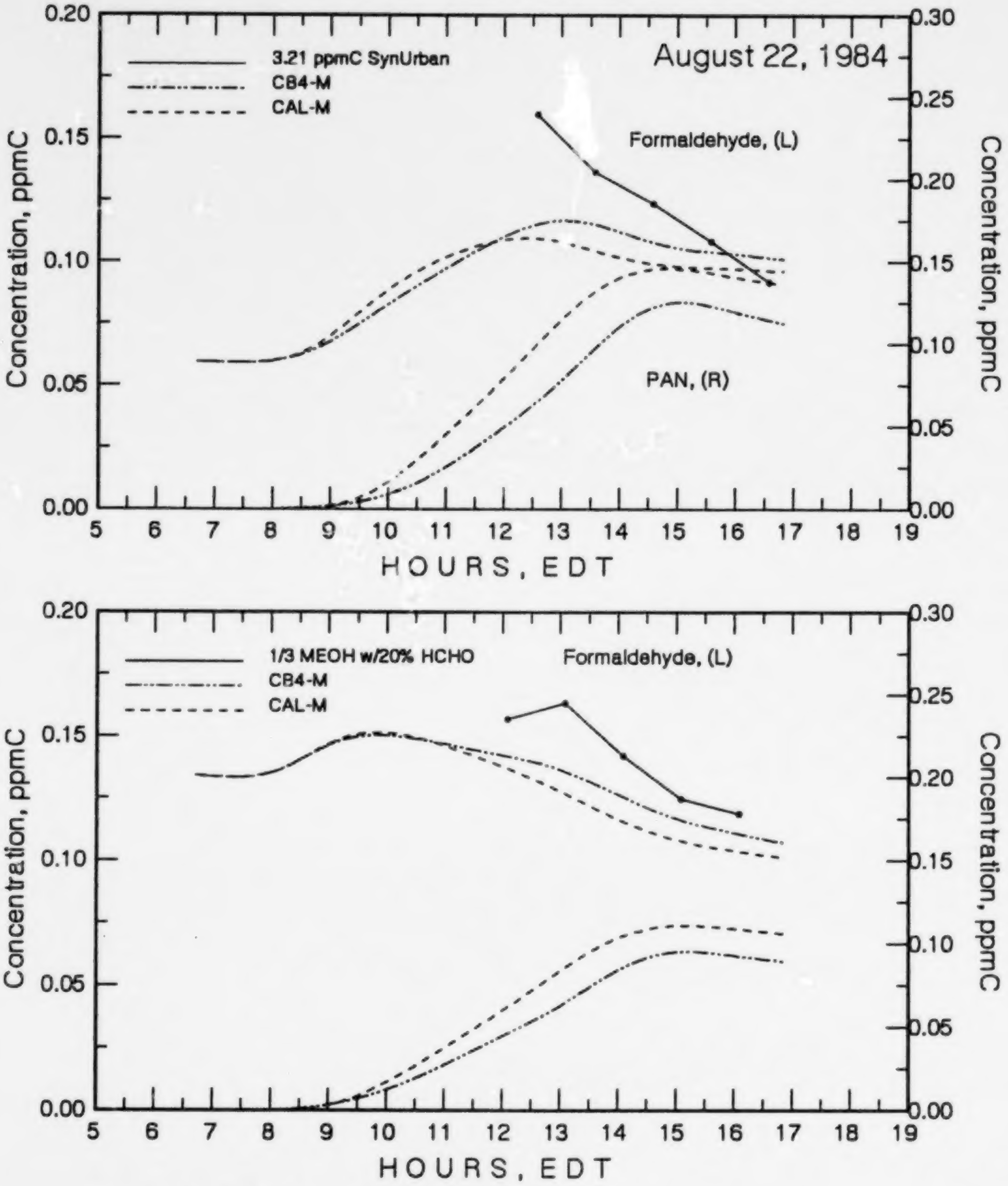


Figure A49. CB4-M and CAL-M Predictions.

August 25, 1984: 1/3 Methanol Substitution w/10% HCHO

Top: 0.72 ppmC SynUrban, 0.29 ppm MEOH, 0.04 ppm HCHO
Bottom: 1.12 ppmC SynUrban

Chamber Observations:

The temperature (Fig. A50) is close to the dewpoint during the early morning hours, and therefore, the timing of the model predictions is expected to be late. There is very little ozone produced on either side of the chamber and NO_x concentrations remain high throughout the day. The methanol substitution decreases the peak ozone concentration from 0.1 ppm to 0.08 ppm.

CB4 and CAL Predictions:

The NO_x crossover points (Fig. A51) predicted by CB4 and CAL are early compared to the observed crossover points. Having expected late crossover predictions, the models appear to be too reactive and too fast.

The decay of toluene (Fig. A52) is tracked well by CB4 and CAL on both sides of the chamber. However, both mechanisms predict much faster ethylene decays than were observed on either side of the chamber. On the substitution side (top), the predicted methanol decay is slower than the observed decay. Thus, the mechanisms are not consuming OH radicals in the correct way; they are too reactive for ethylene and not reactive enough for methanol.

As expected, CB4 and CAL over predict the amount of ozone produced (Fig. A51) on both sides of the chamber with P/O ratios greater than 2. Both mechanisms adequately predict the relative change due to the methanol substitution.

CB4 and CAL under predict the formaldehyde concentration profiles (Fig. A53) on both sides of the chamber with P/O ratios of about 0.7. PAN concentrations are over predicted by CB4 with P/O ratios of 3 and 4 for the substitution side (top) and the control side (bottom), respectively. CAL performs worse generating P/O ratios of 6 and 7, respectively.

CIT Predictions:

The NO_x crossover points (Fig. A54) predicted by the CIT mechanisms are well timed compared to the observed crossover points.

The hydrocarbon decay profiles (Fig. A55) predicted by the CIT mechanisms are similar to those predicted by CB4 and CAL.

CIT-1 produces ozone concentration profiles (Fig. A54) similar to those produced by CB4 and CAL, over predicting the peak concentrations with P/O ratios greater than 2. CIT-2, on the other hand, produces ozone concentration profiles very close to the observed profiles, with P/O ratios less than 1.2.

Both CIT mechanisms under predict the formaldehyde concentration profiles (Fig. A56) on both sides of the chamber. CIT-1 produces the same final concentrations as CB4 and CAL, with P/O ratios of about 0.7. CIT-2 produces lower profiles with P/O ratios of about 0.5. The PAN concentration profiles produced by the CIT mechanisms stradle the observed profiles. CIT-2 tracks the observed profile on the substitution side (top) very well and over predicts the profile on the control side (bottom). CIT-1 under predicts the profile on both sides of the chamber.

Wall Model Effects:

Switching to Killus's wall model (Figs. A57-9) improves the performance of CB4 and CAL in predicting ozone, formaldehyde, and PAN concentrations. Eliminating the wall reactions (Figs. A60-2) improves the performance of CB4 and CAL in predicting ozone and PAN concentrations but decreases the performance in predicting formaldehyde concentrations.

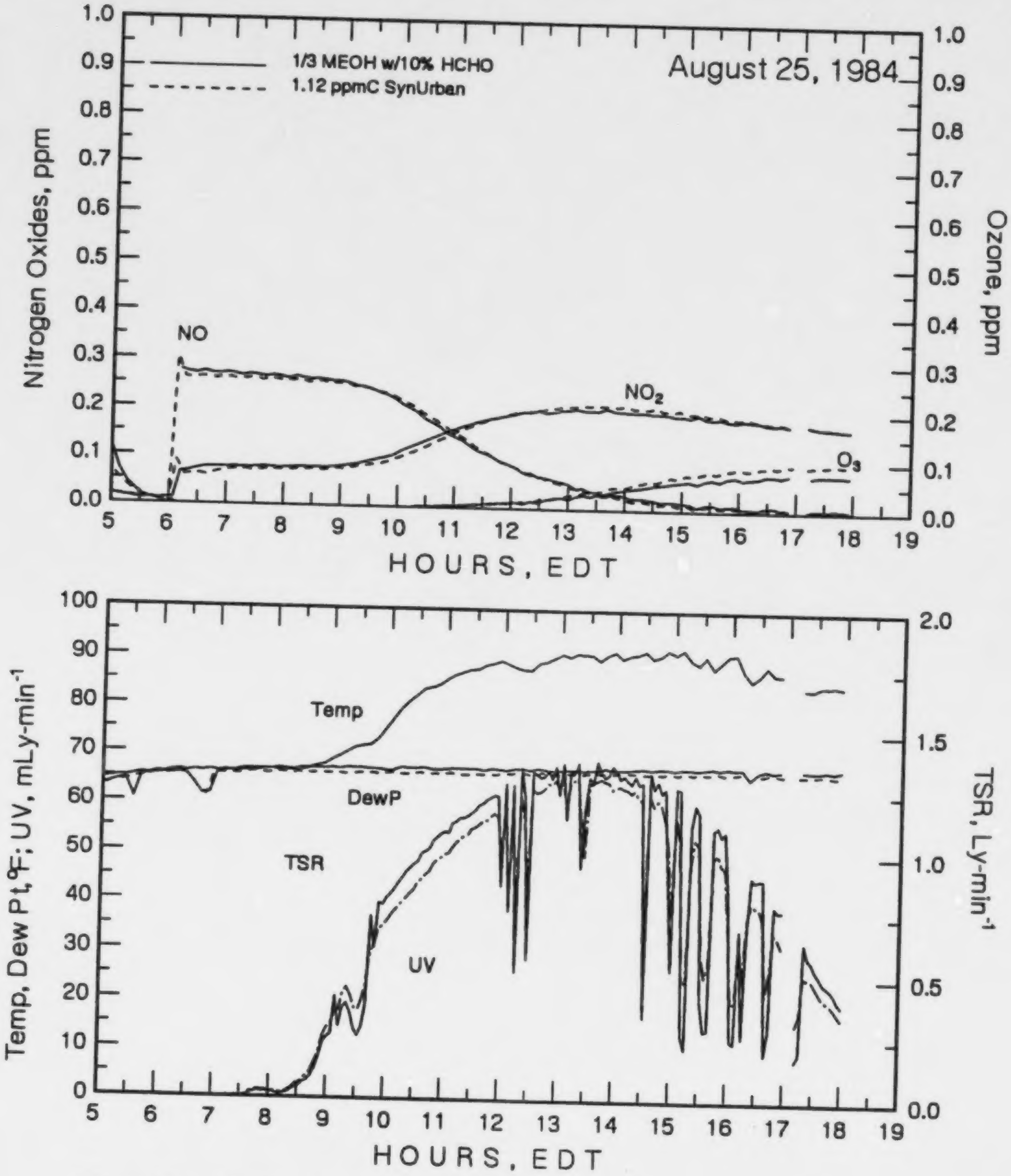


Figure A50. Chamber Observations.

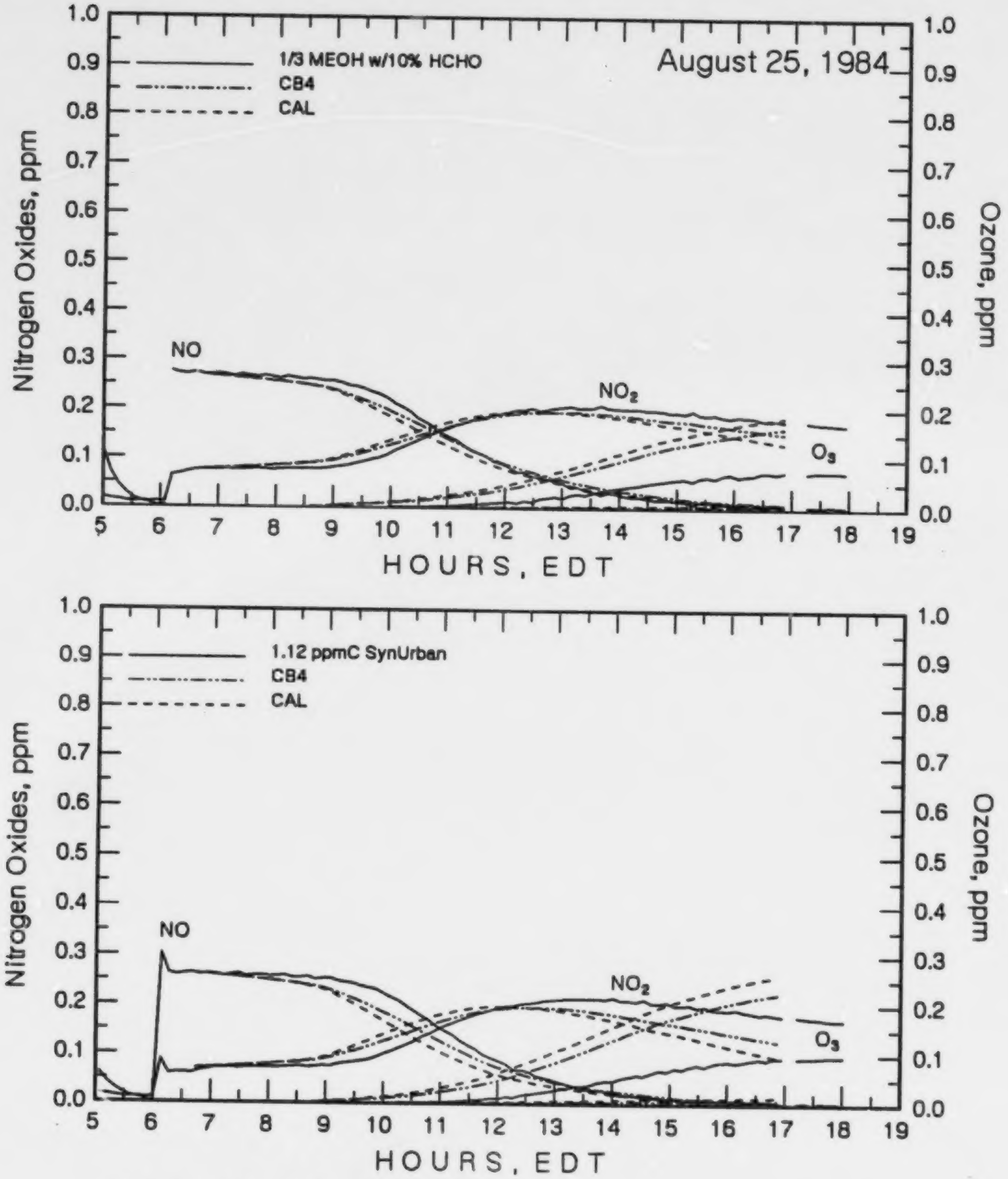


Figure A51. CB4 and CAL Predictions.

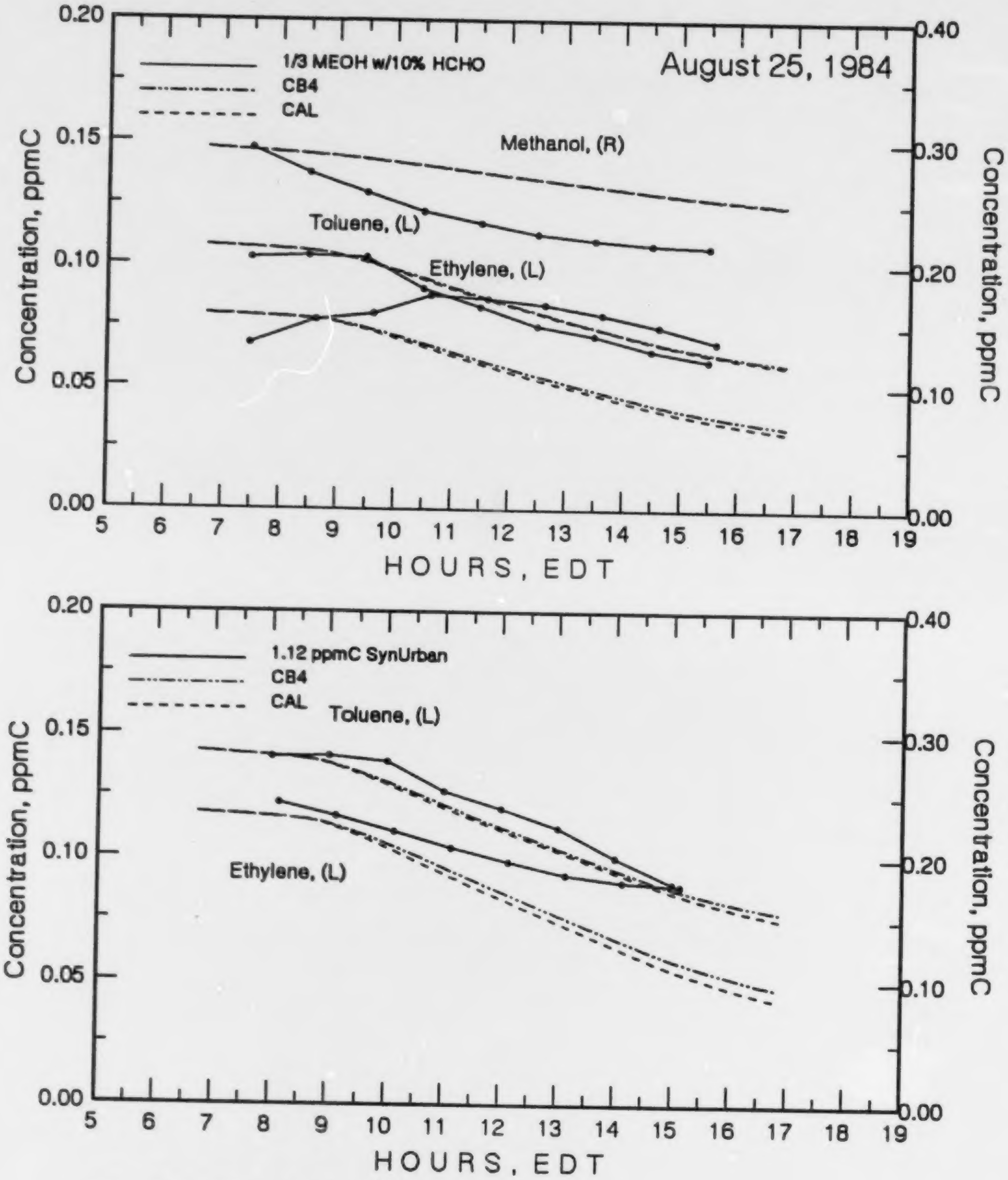


Figure A52. CB4 and CAL Predictions.

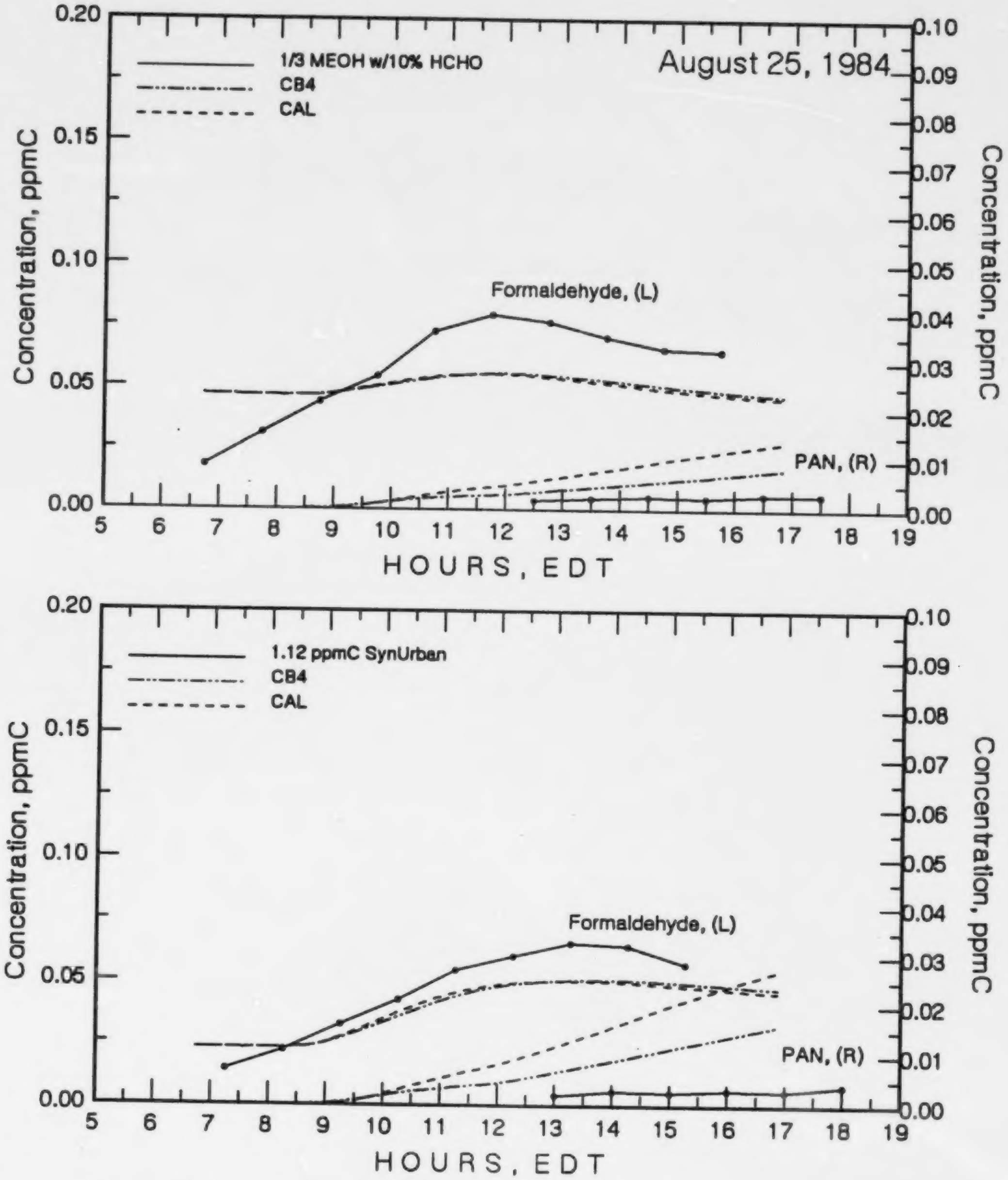
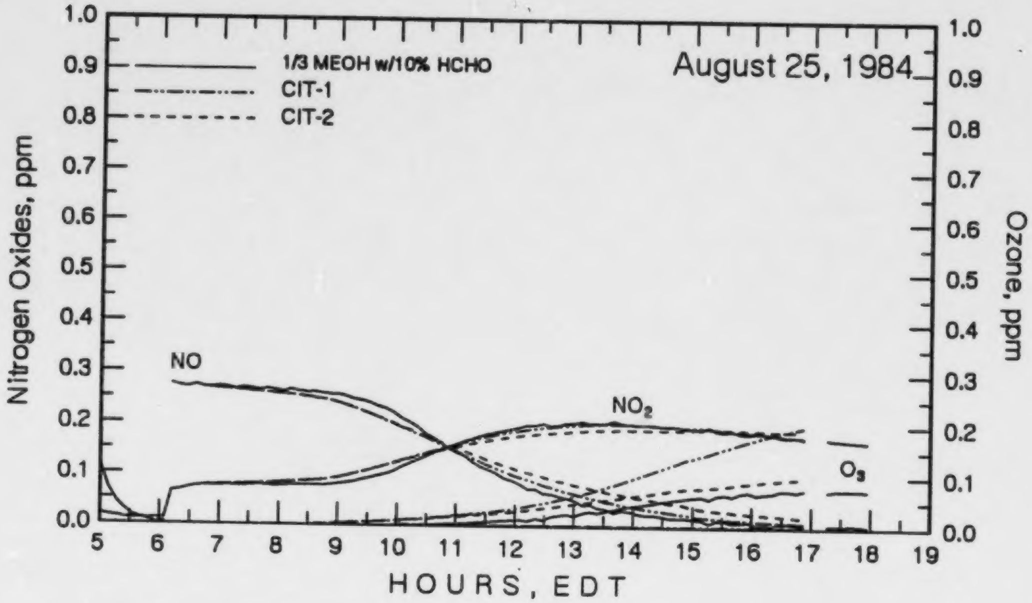


Figure A53. CB4 and CAL Predictions.



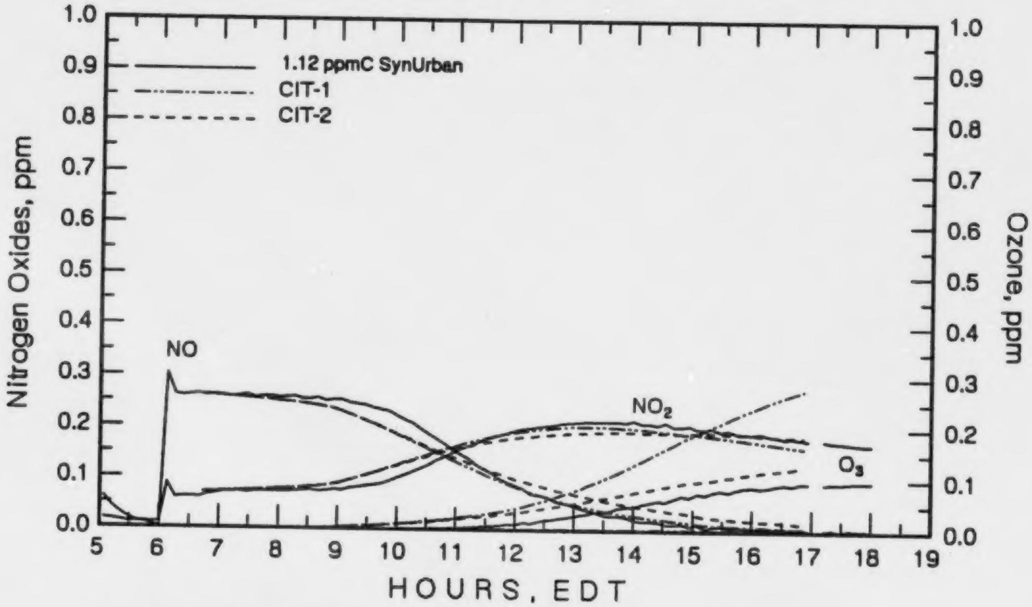


Figure A54. CIT Predictions.

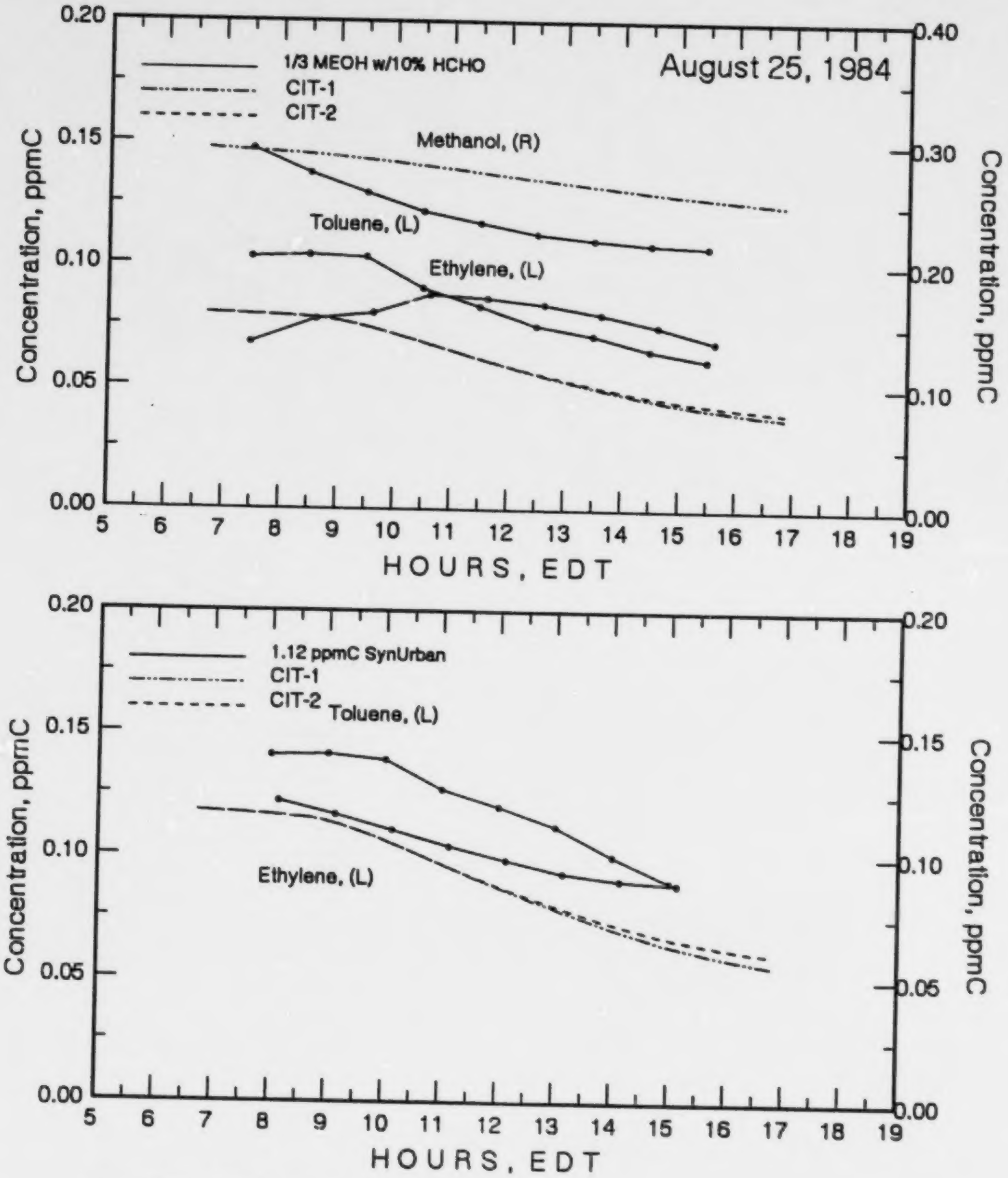


Figure A55. CIT Predictions.

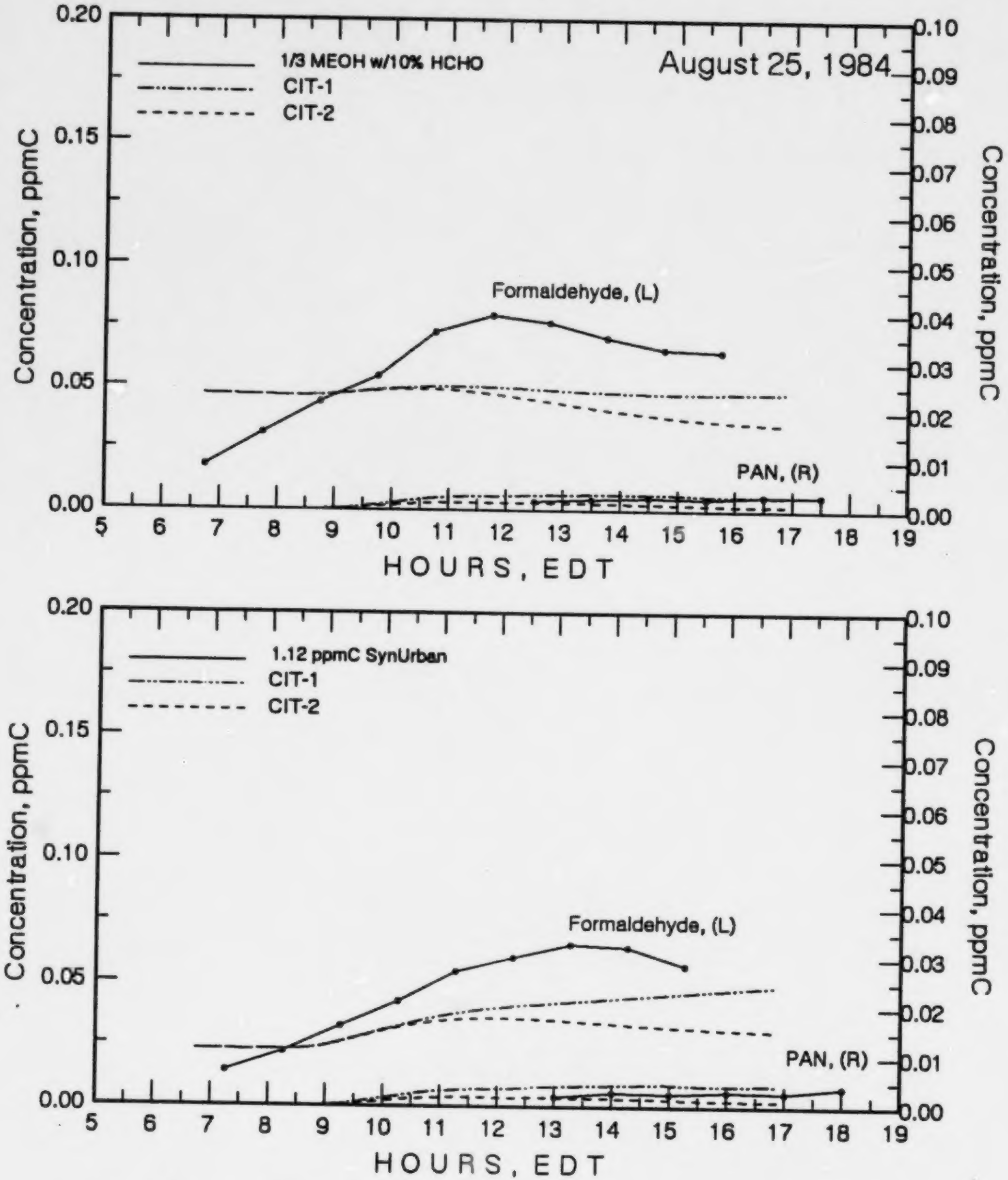


Figure A56. CIT Predictions.

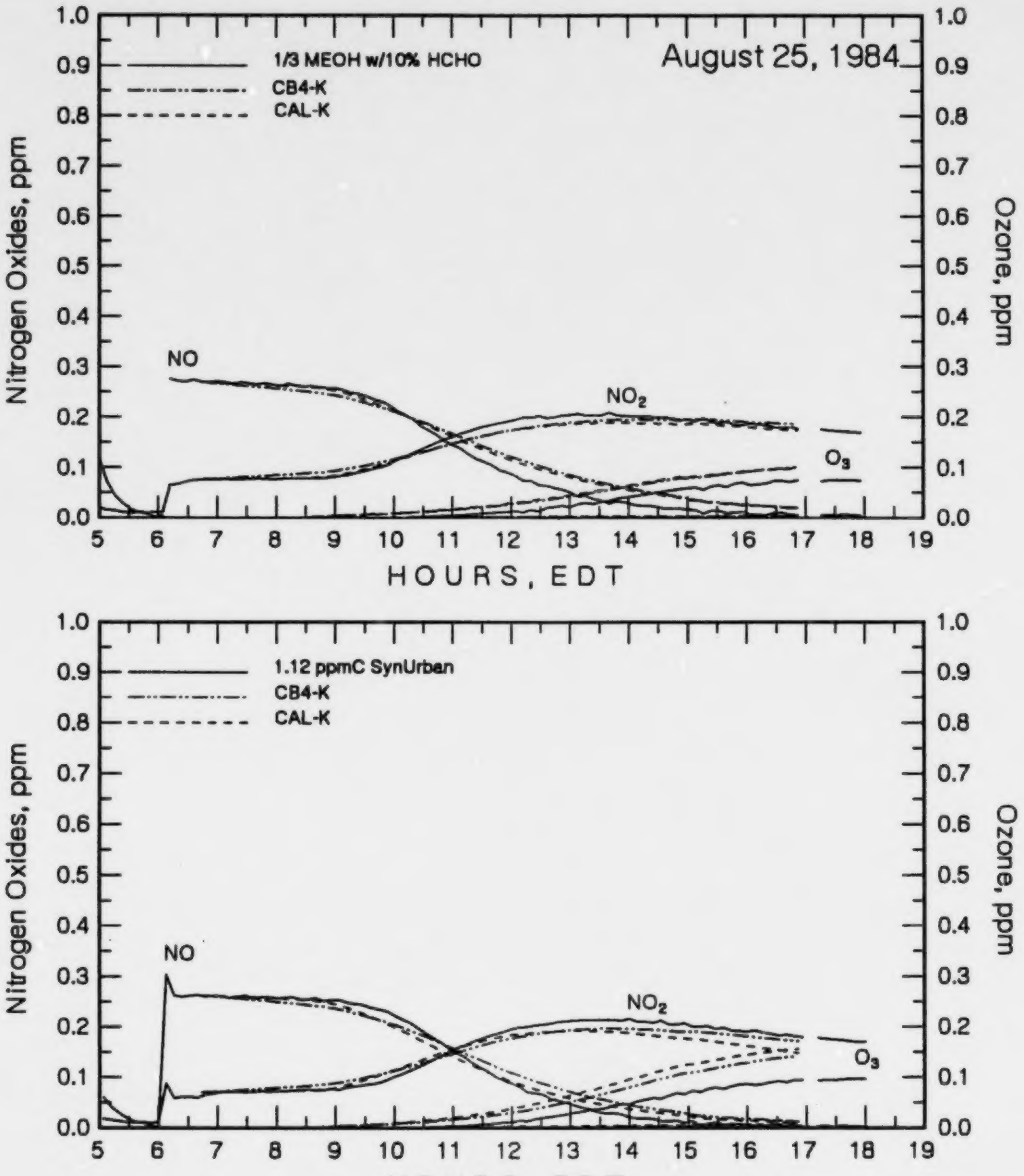
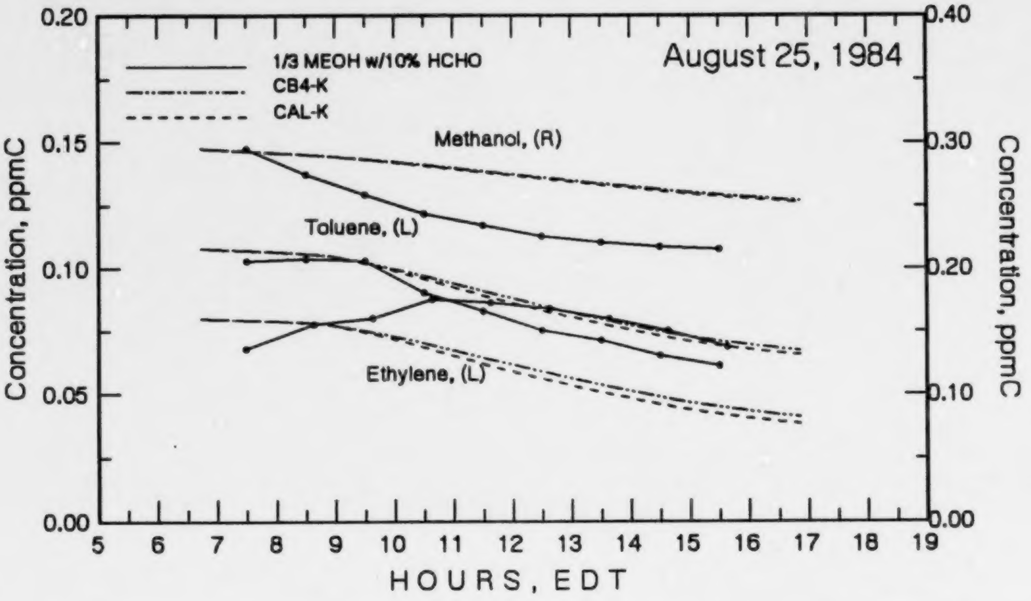


Figure A57. CB4-K and CAL-K Predictions.



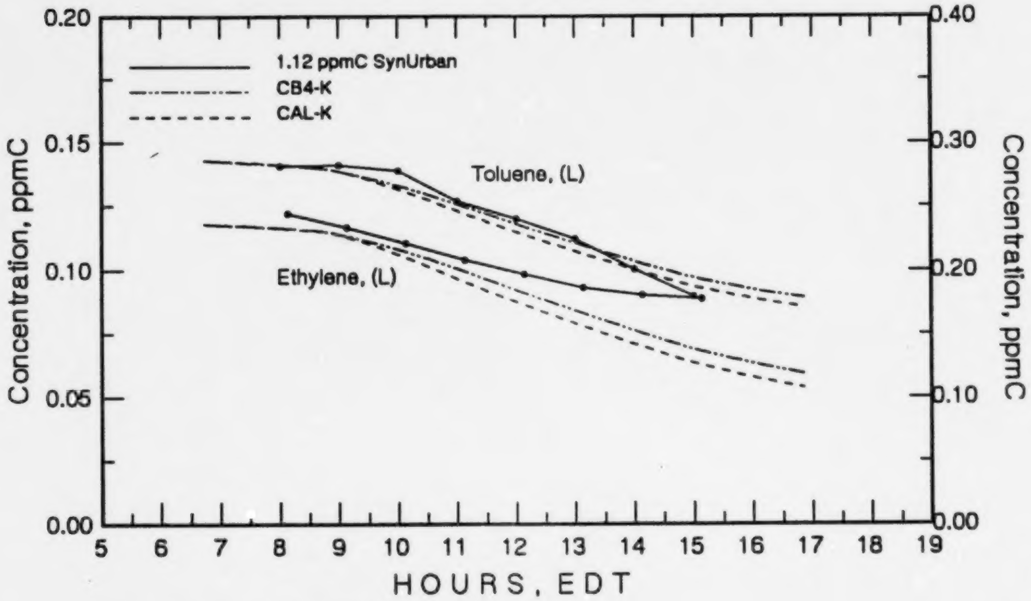


Figure A58. CB4-K and CAL-K Predictions.

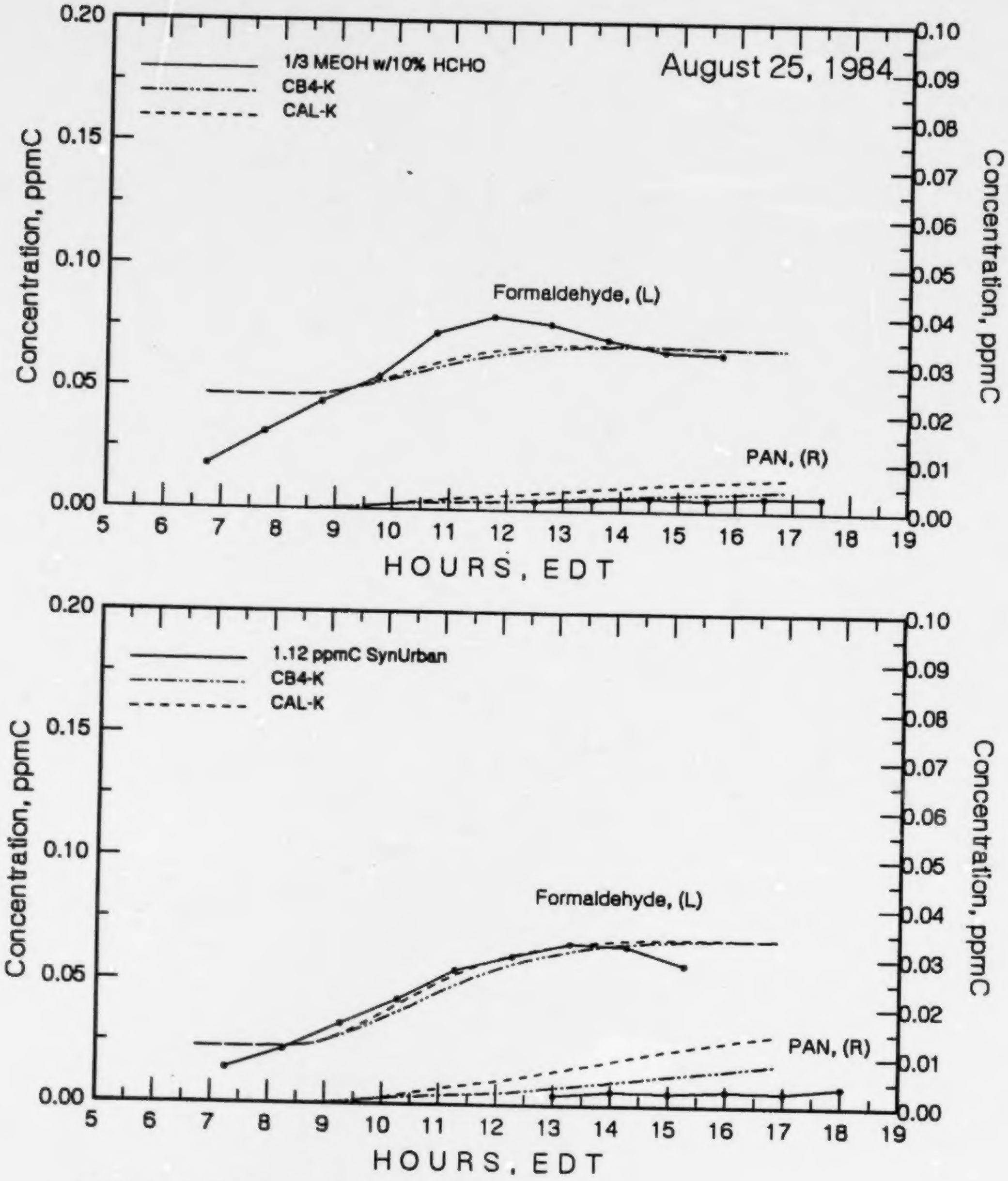


Figure A59. CB4-K and CAL-K Predictions.

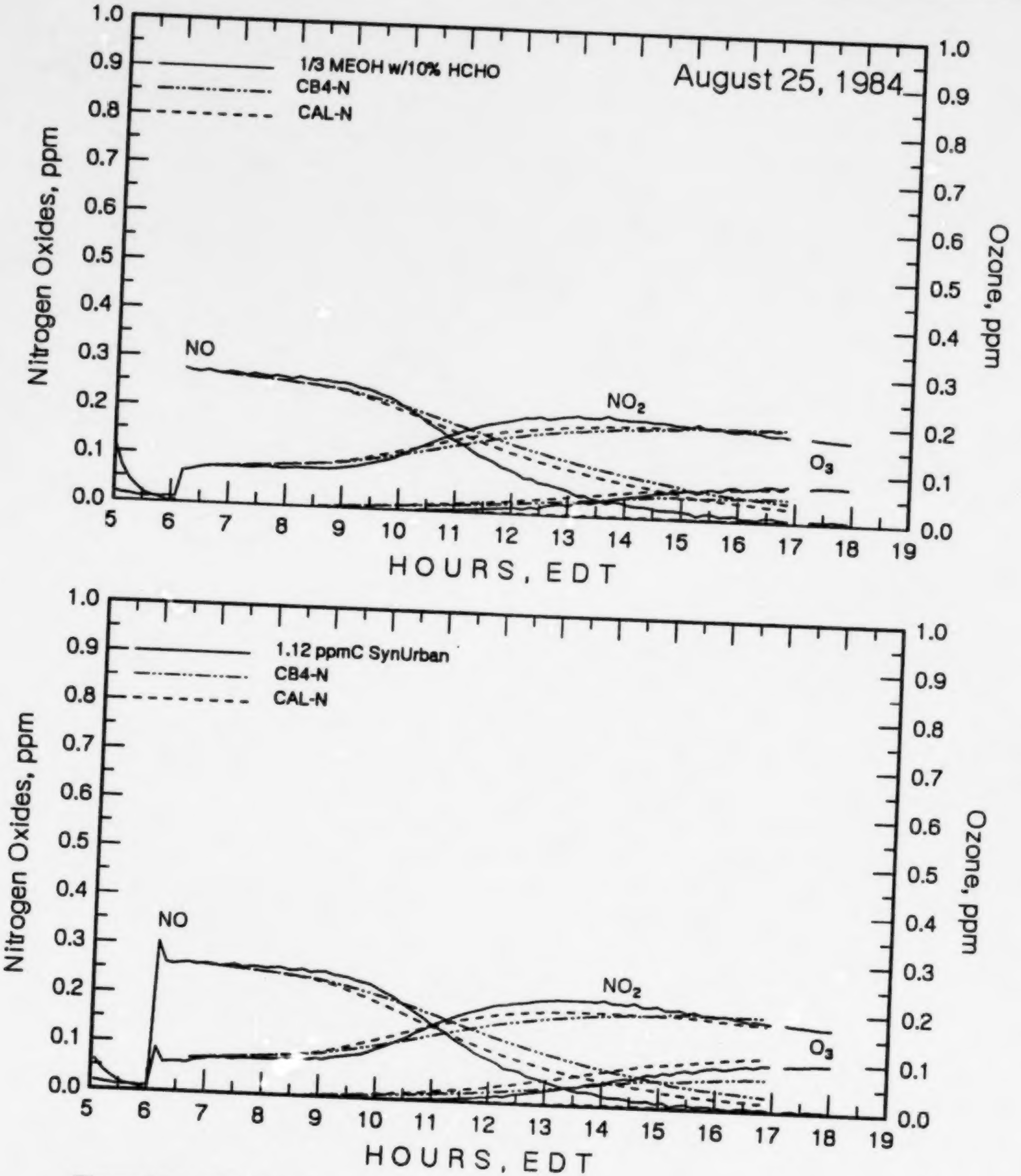
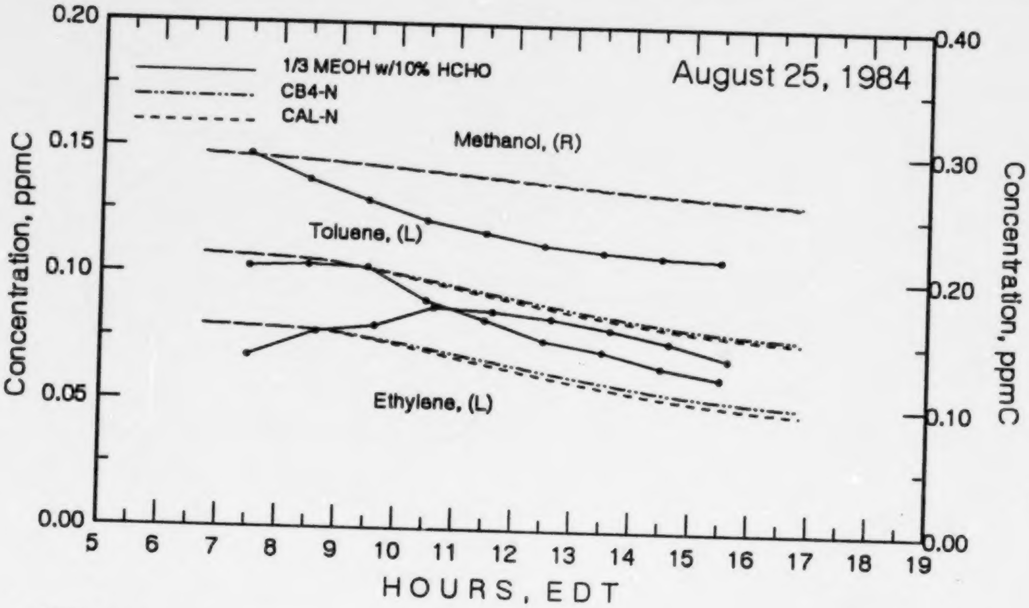


Figure A60. CB4-N and CAL-N Predictions.



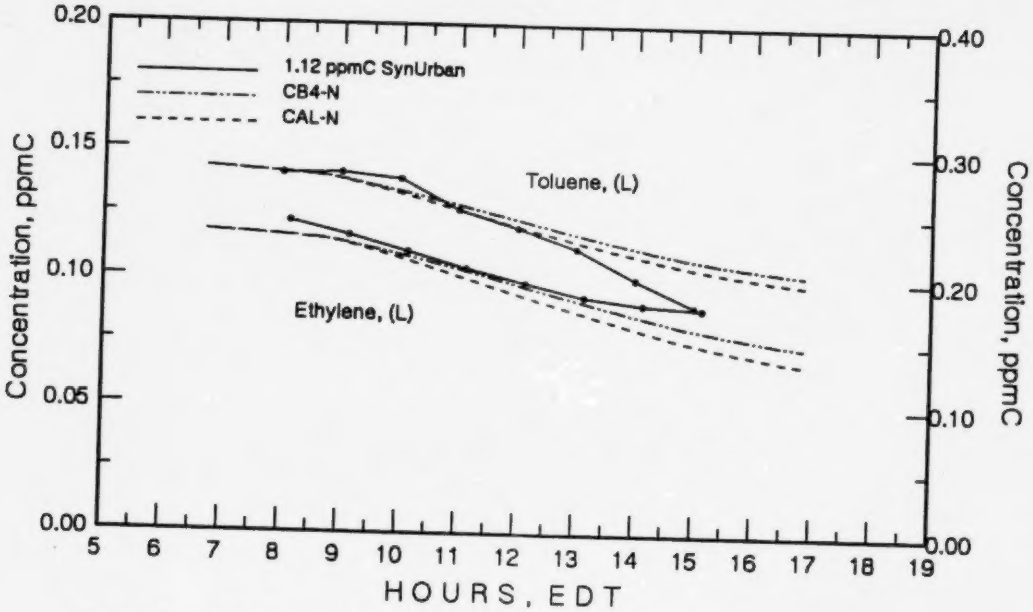
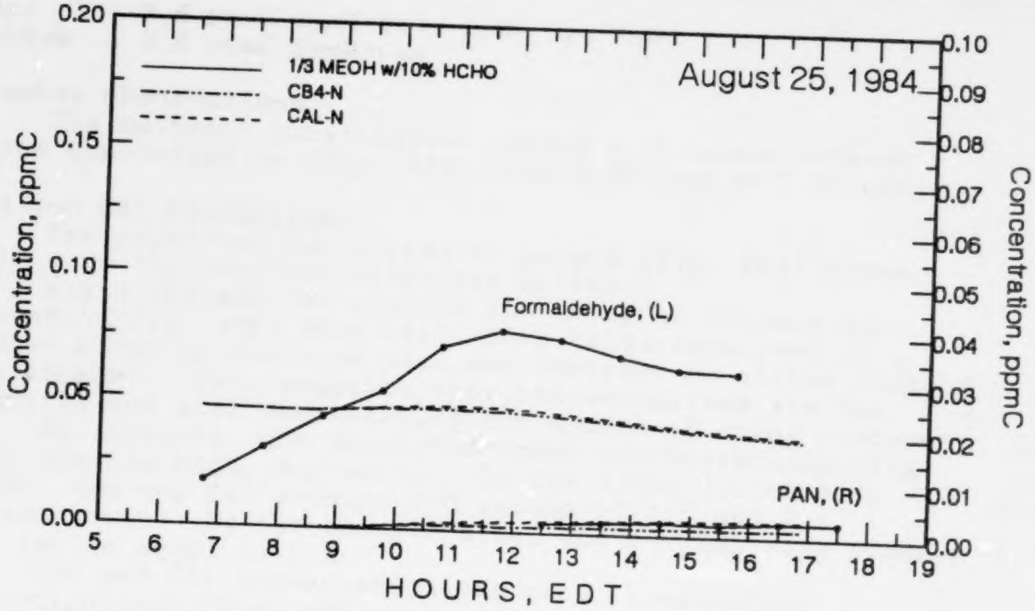


Figure A61. CB4-N and CAL-N Predictions.



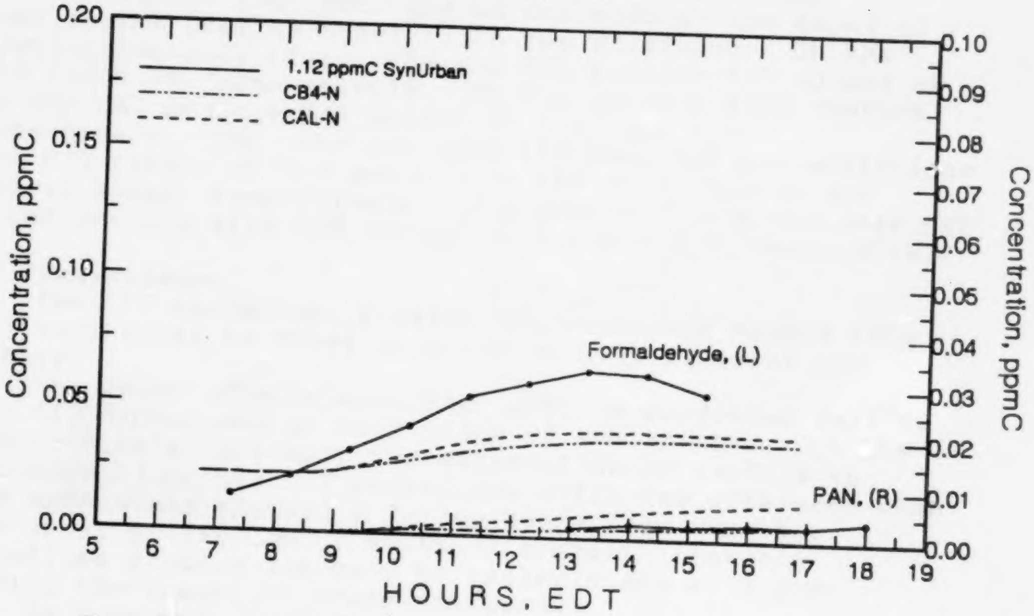


Figure A62. CB4-N and CAL-N Predictions.

September 1, 1984: 1/3 Methanol Substitution

Top: 2.6 ppmC SynUrban, 0.97 ppm MEOH
Bottom: 3.3 ppmC SynUrban

Chamber Observations:

The methanol substitution caused a decrease in peak ozone concentration (Fig. A63) from 0.65 ppm to 0.55 ppm.

CB4 and CAL Predictions:

The predicted NOx crossover points (Fig. A64) agree well with the observed crossover points.

While CB4 and CAL predict the decay of toluene and methanol (Fig. A65) very well, both mechanisms predict a faster decay of ethylene than was observed on either side of the chamber. This suggests that the mechanisms are too reactive and will over predict the amount of ozone produced.

As expected, the predicted ozone concentrations (Fig. A64) are too high, too early. On the substitution side (top), CB4 and CAL produce P/O ratios of 1.5 and 1.4, respectively. On the control side, CB4 and CAL both produce P/O ratios equal to 1.2.

CB4 and CAL underpredict the peak formaldehyde concentrations (Fig. A66) and do not predict the decay of formaldehyde that is observed in the afternoon. On the substitution side (top), CB4 and CAL produce P/O ratios of 0.88 and 0.75, respectively. On the control side (bottom), CB4 and CAL produce P/O ratios of 0.75 and 0.7, respectively. CAL over predicts the peak PAN concentrations with P/O ratios of 3.8 and 2.9 on the substitution and control sides, respectively. CB4 over predicts the peak PAN concentrations with P/O ratios of 3.3 and 2.5, respectively.

CIT Predictions:

The CIT mechanisms predict NO_x crossover points (Fig. A67) very close to those observed on both sides of the chamber.

The decay of ethylene (Fig. A68) is predicted well by both CIT mechanisms on both sides of the chamber. On the substitution side (top), the methanol decay profile is tracked well by the CIT mechanisms until the afternoon when both mechanisms predict a faster decay than was observed. This under prediction of methanol suggests that the mechanisms produce too many OH radicals and will over predict the amount of ozone produced.

As expected, both CIT mechanisms over predict the ozone concentration profiles (Fig. A67). The predictions of CIT-1 are much too high. CIT-2 over predicts with P/O ratios of 1.25 and 1.5 on the substitution (top) and control (bottom) sides, respectively.

The formaldehyde concentration profiles (Fig. A69) predicted by CIT-1 are wrong in that they continue to increase throughout the afternoon. The formaldehyde concentration profiles predicted by CIT-2 underpredict the observed profile, but have final concentrations similar to those predicted by CB4 and CAL. Both CIT mechanisms under predict PAN concentrations on both sides of the chamber.

Wall Model Effects:

Switching to Killus's wall model (Figs. A70-2) improves the performance of CB4 and CAL in predicting ozone, formaldehyde, and PAN concentrations. Overall, eliminating the wall reactions (Figs. A73-5) yields the best model predictions.

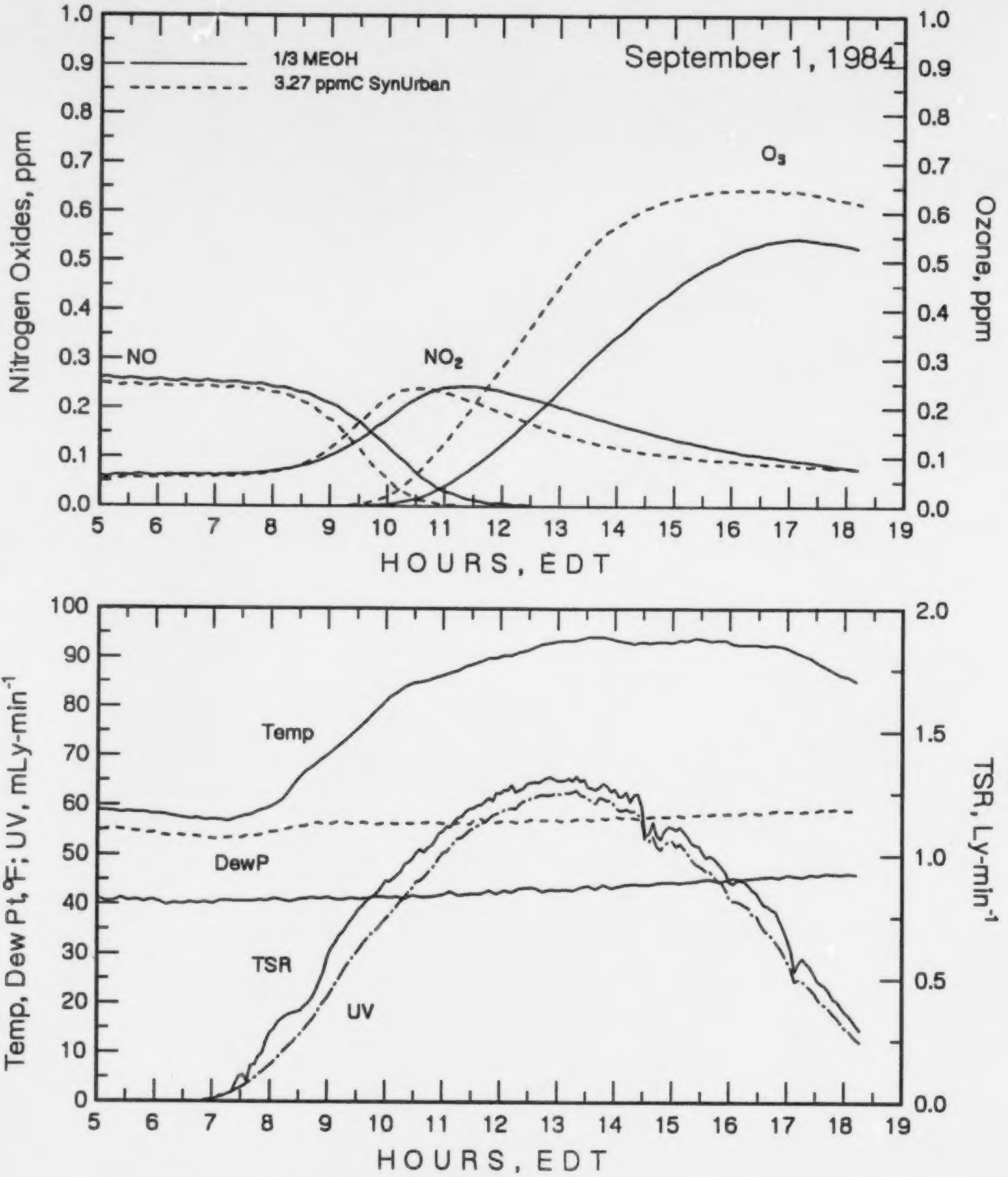
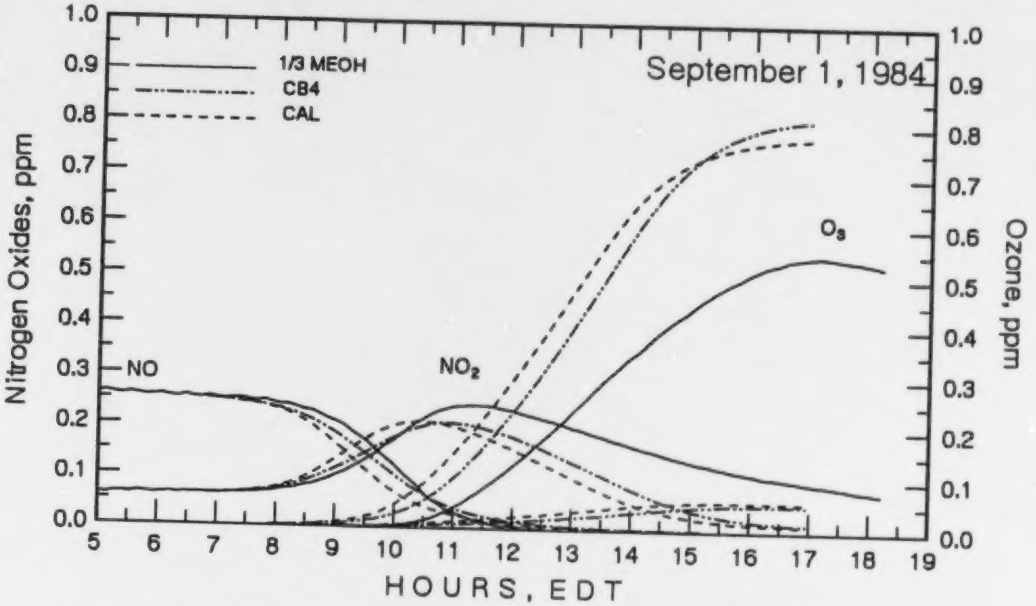


Figure A63. Chamber Observations.



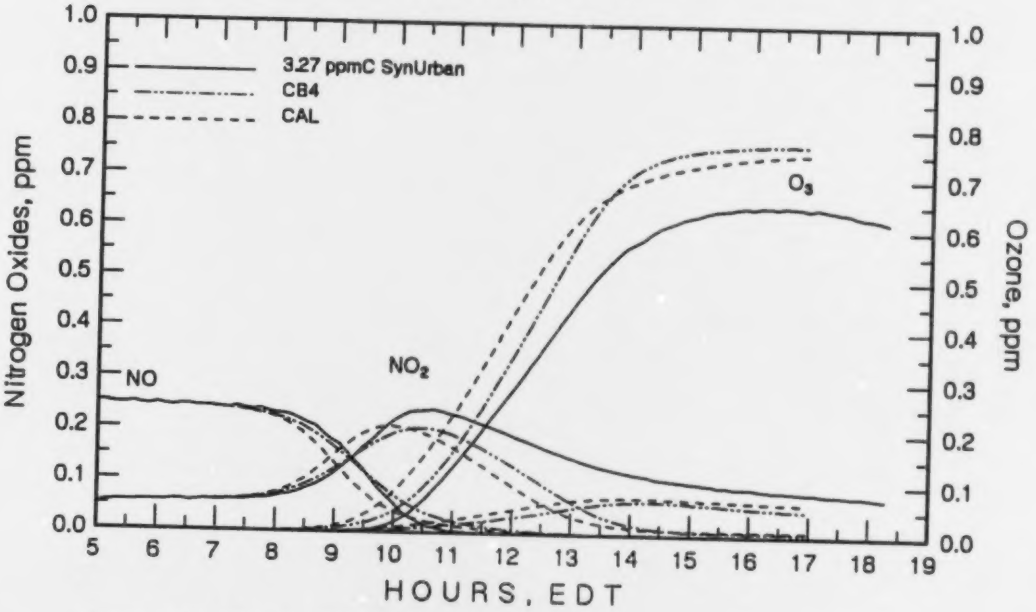


Figure A64. CB4 and CAL Predictions.

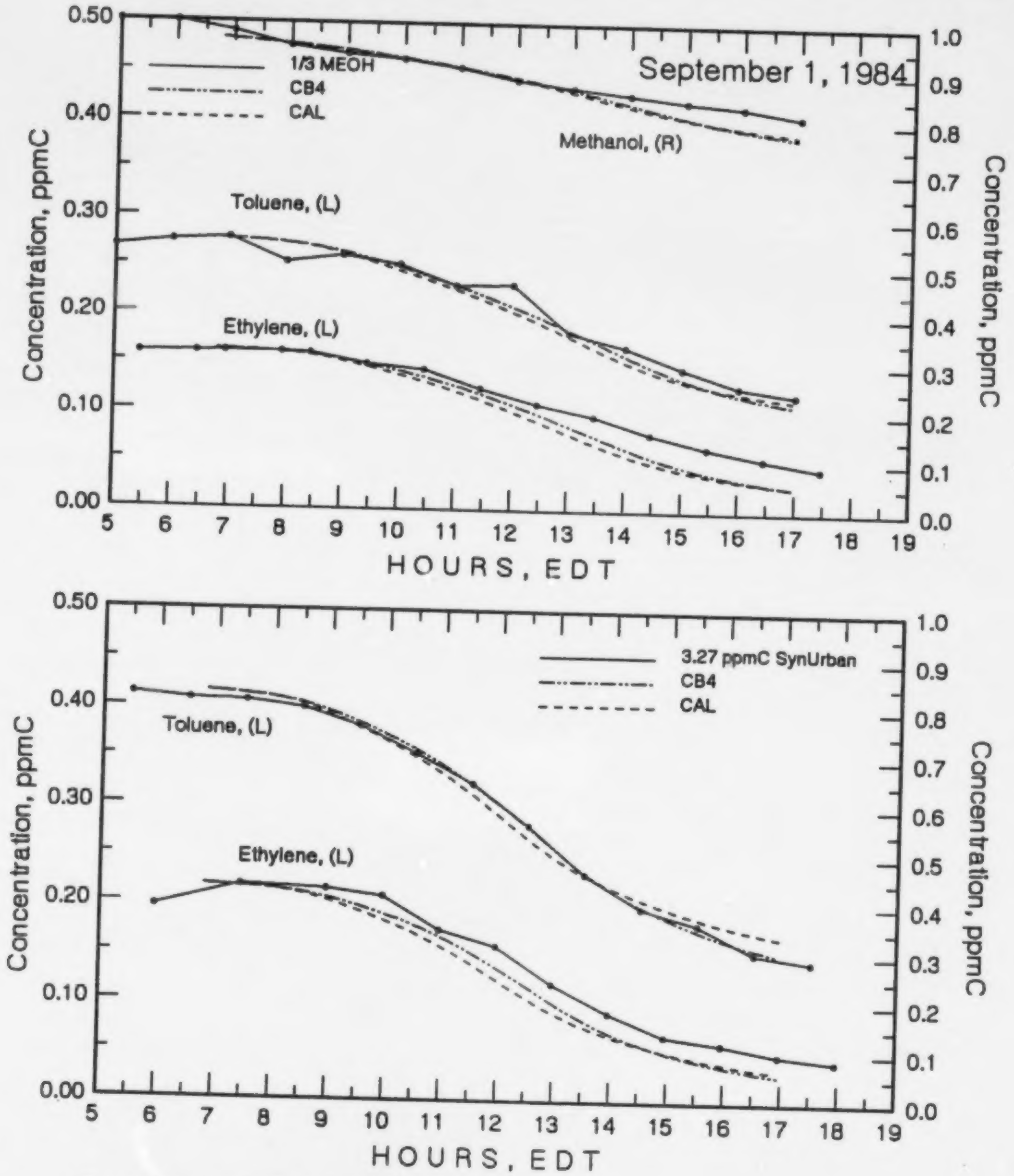


Figure A65. CB4 and CAL Predictions.

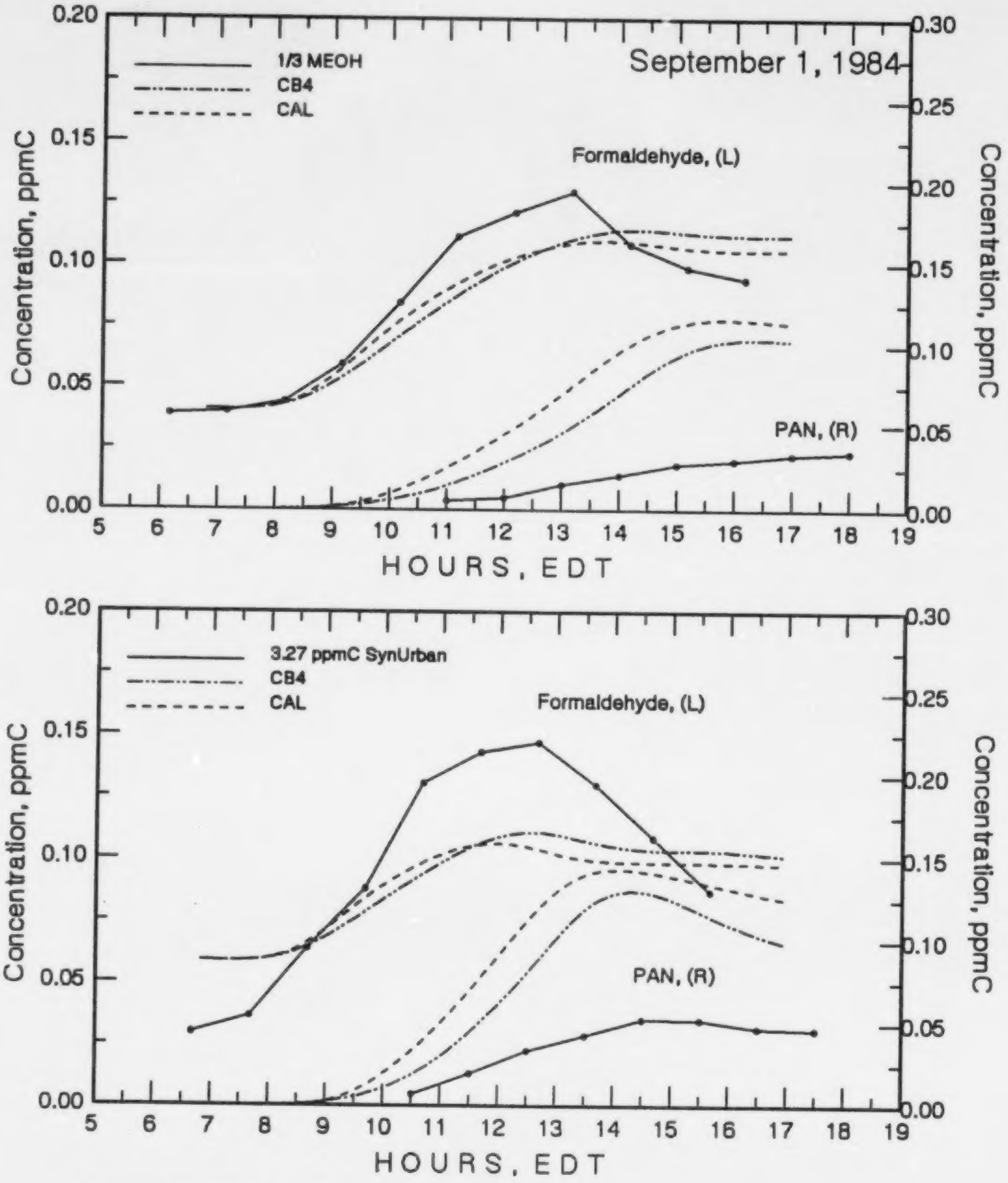
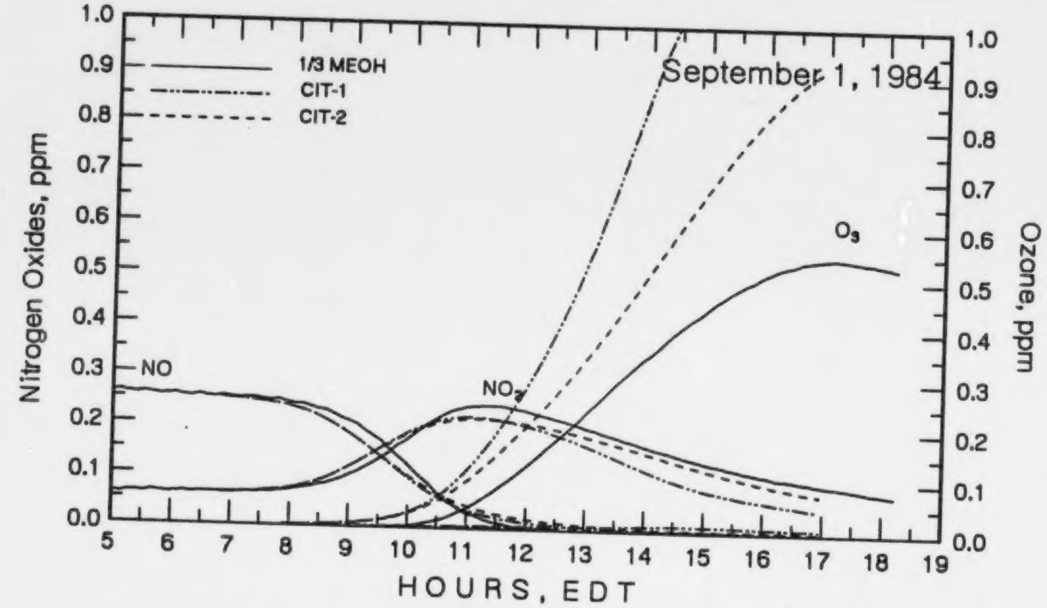


Figure A66. CB4 and CAL Predictions.



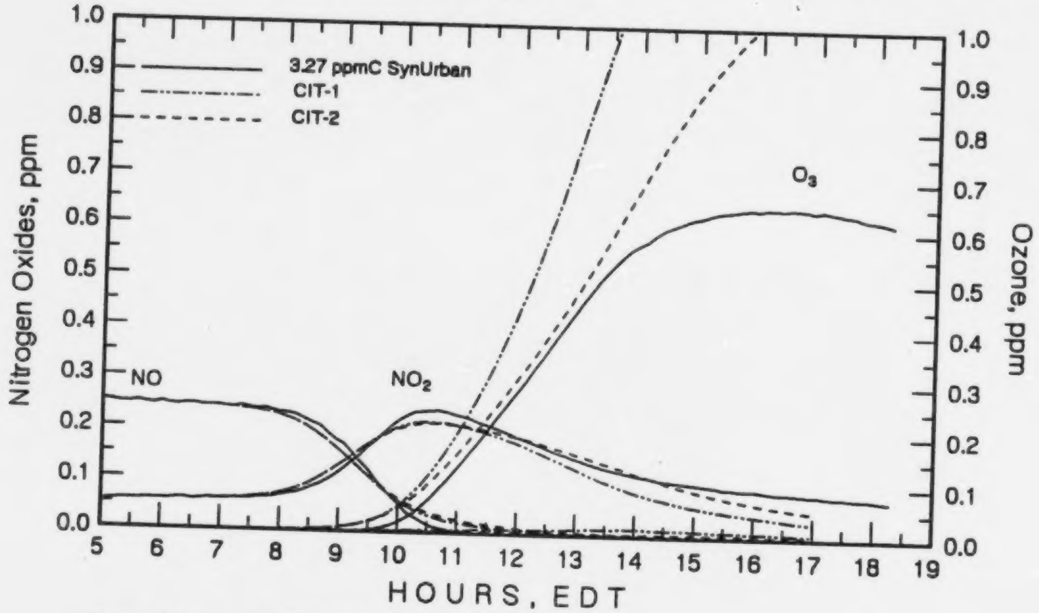


Figure A67. CIT Predictions.

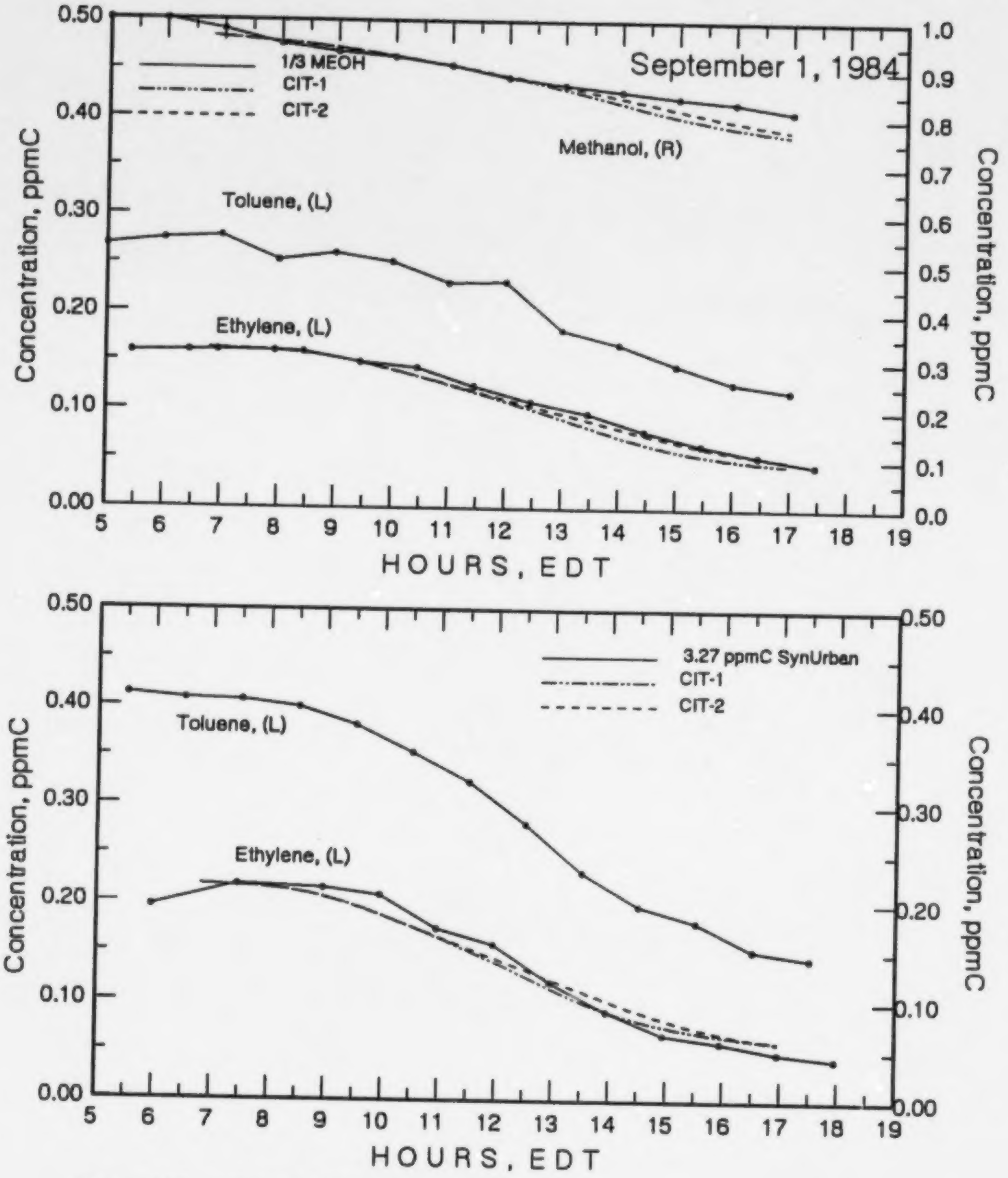


Figure A68. CIT Predictions.

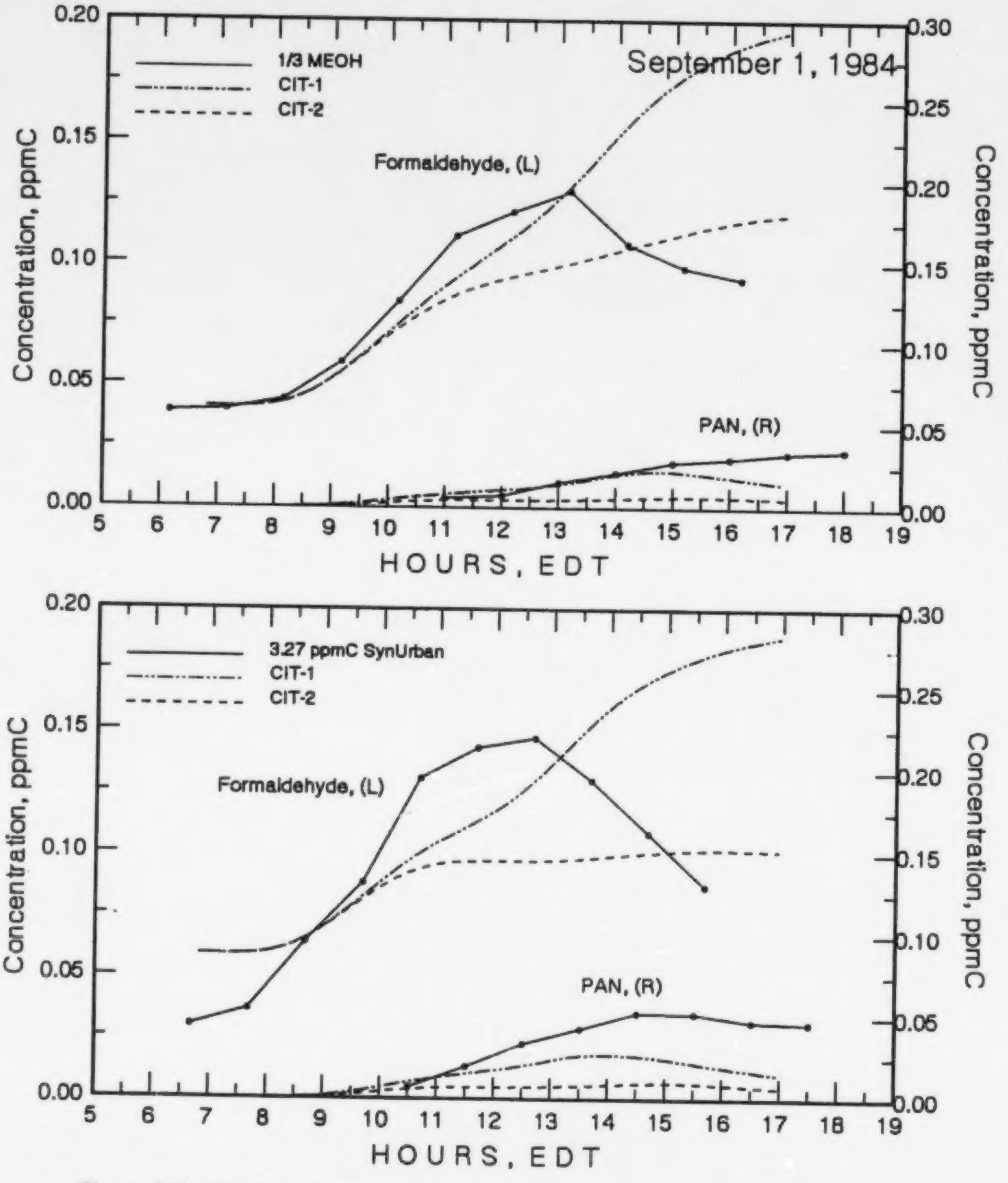
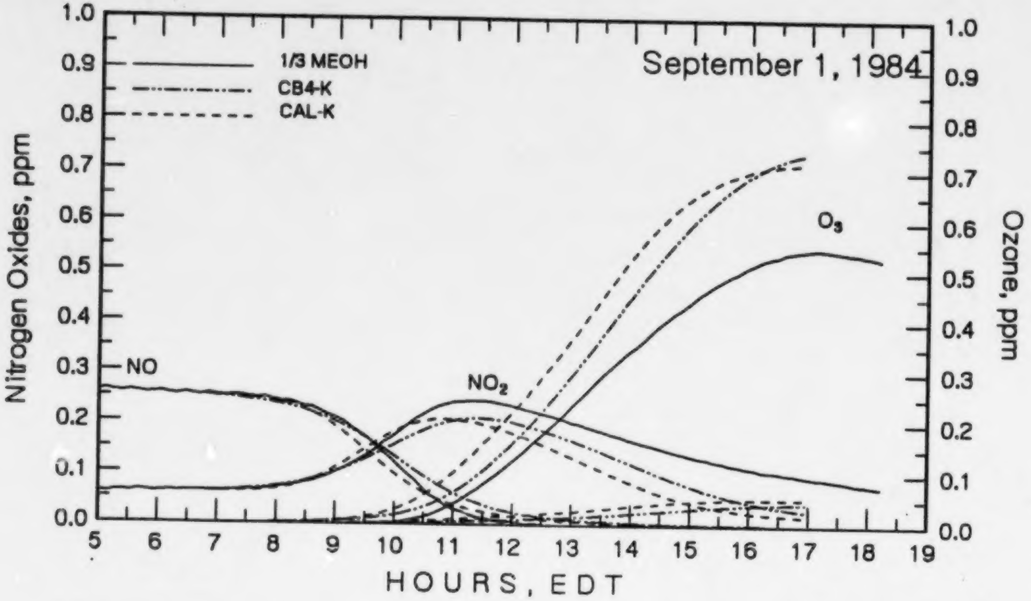


Figure A69. CIT Predictions.



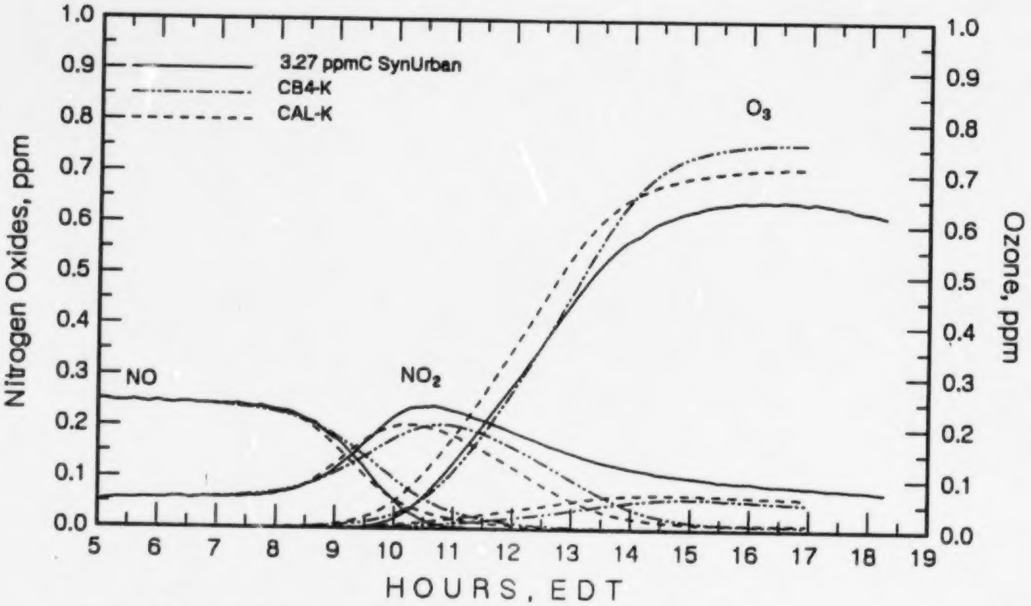


Figure A70. CB4-K and CAL-K Predictions.

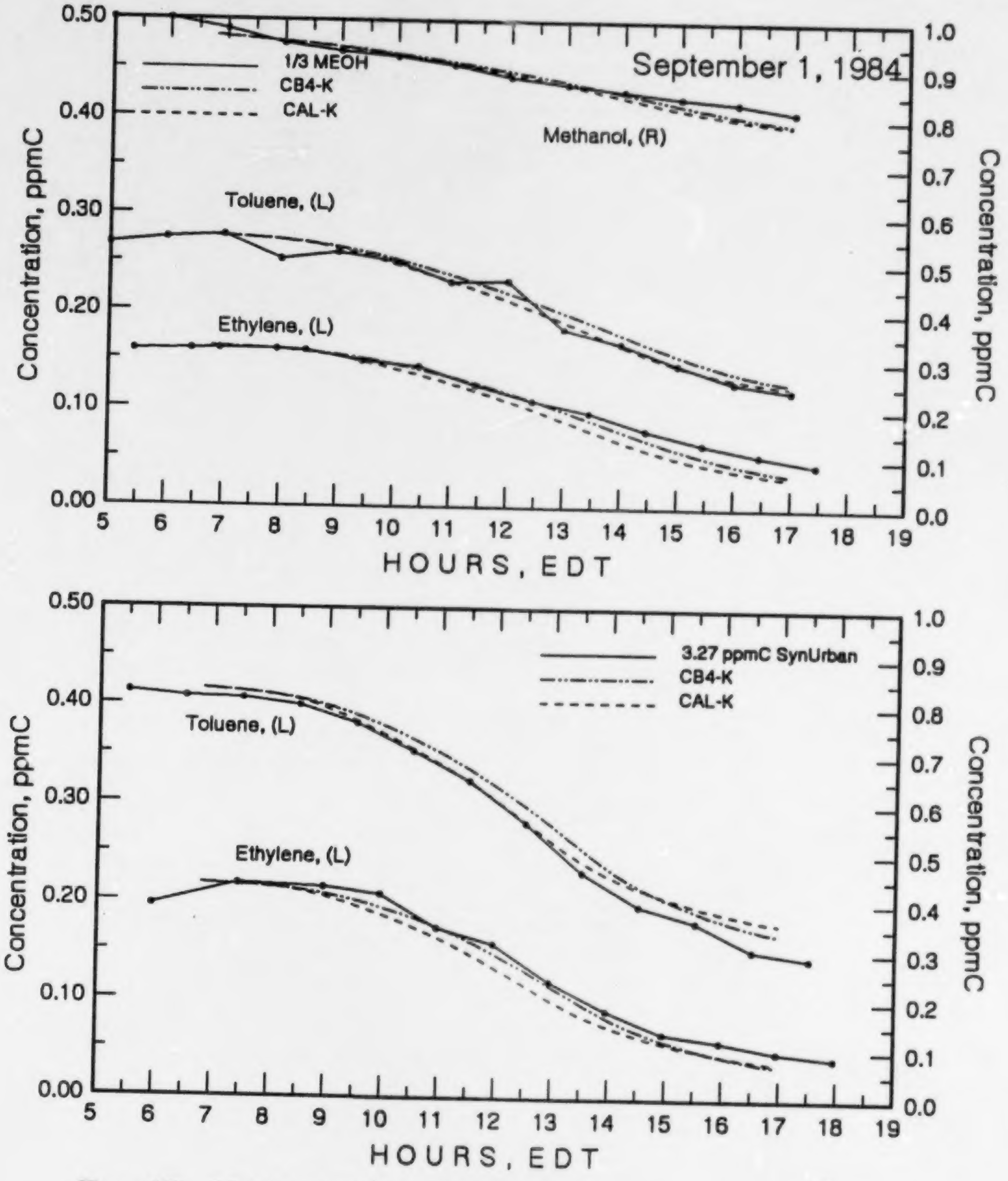


Figure A71. CB4-K and CAL-K Predictions.

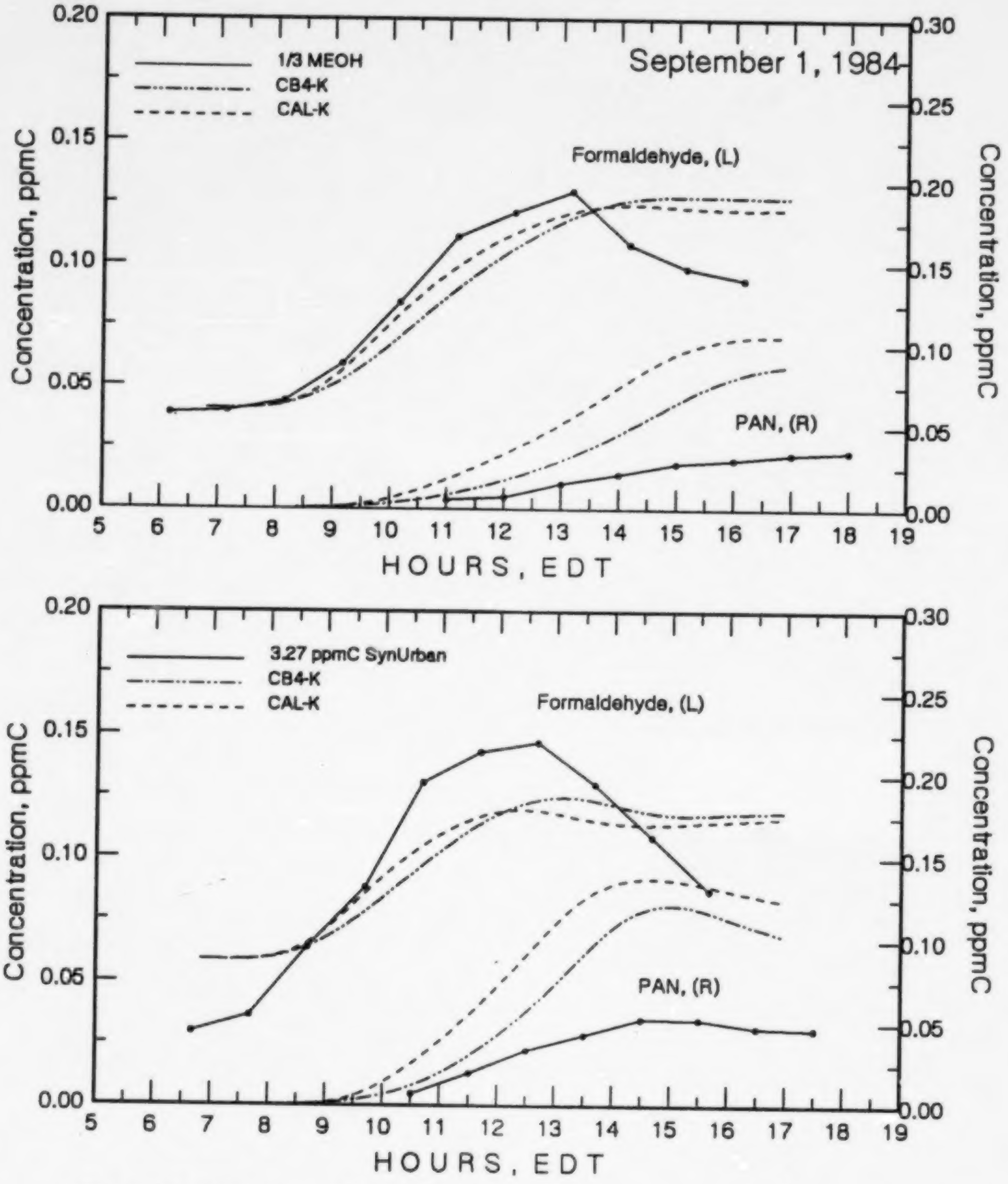


Figure A72. CB4-K and CAL-K Predictions.

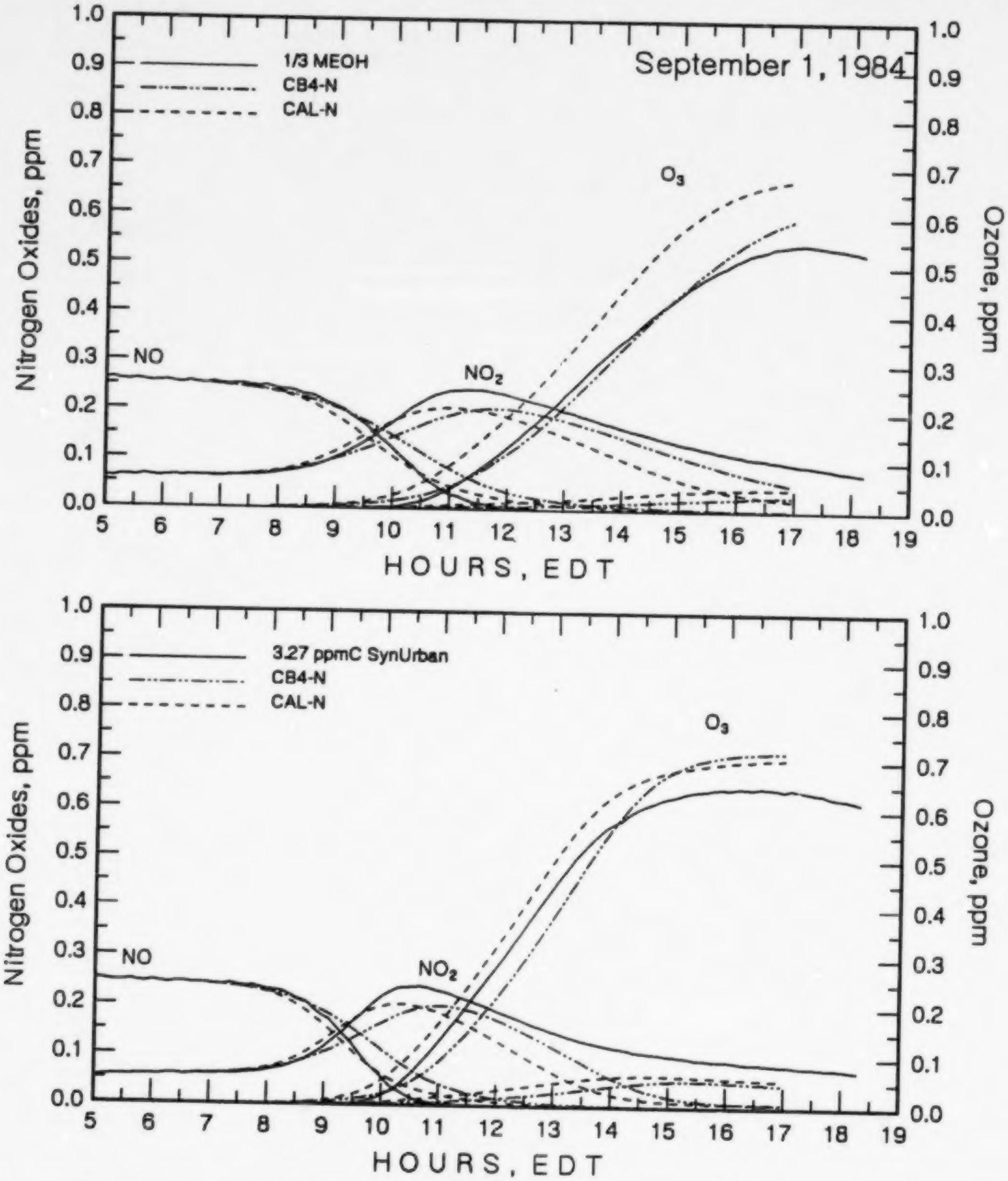
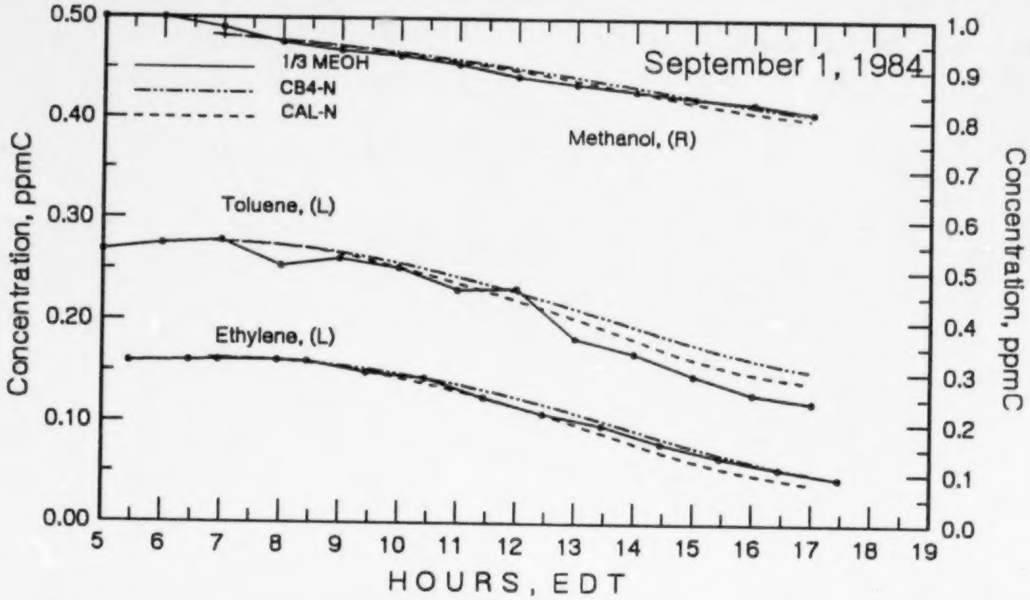


Figure A73. CB4-N and CAL-N Predictions.



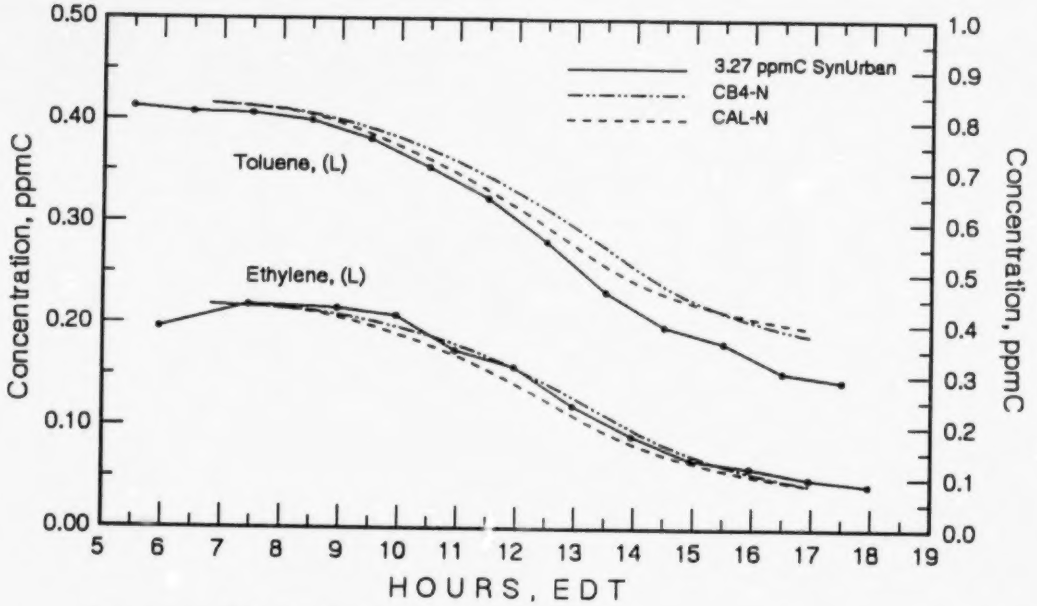
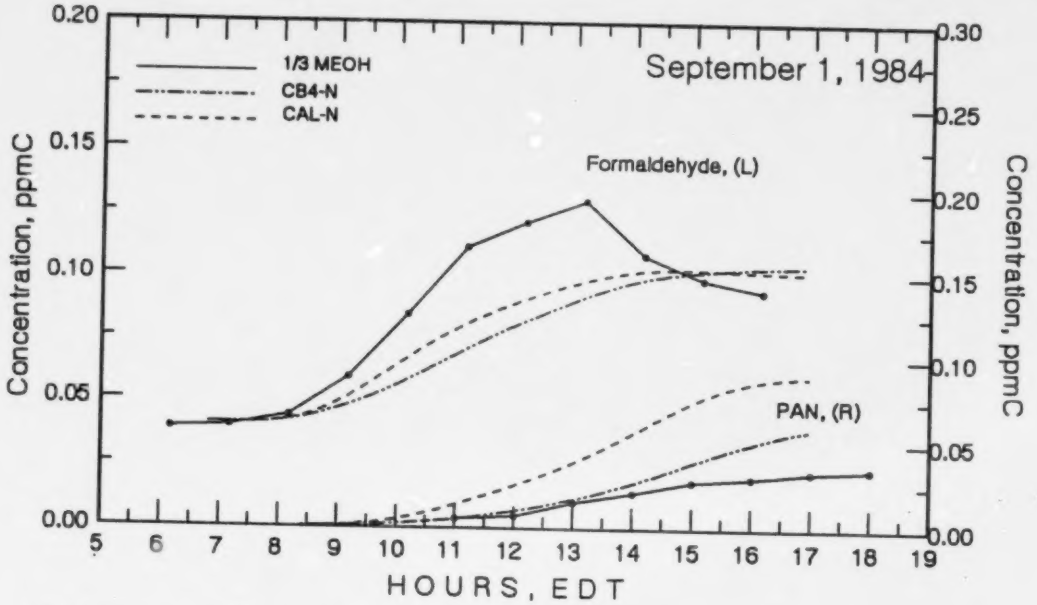


Figure A74. CB4-N and CAL-N Predictions.



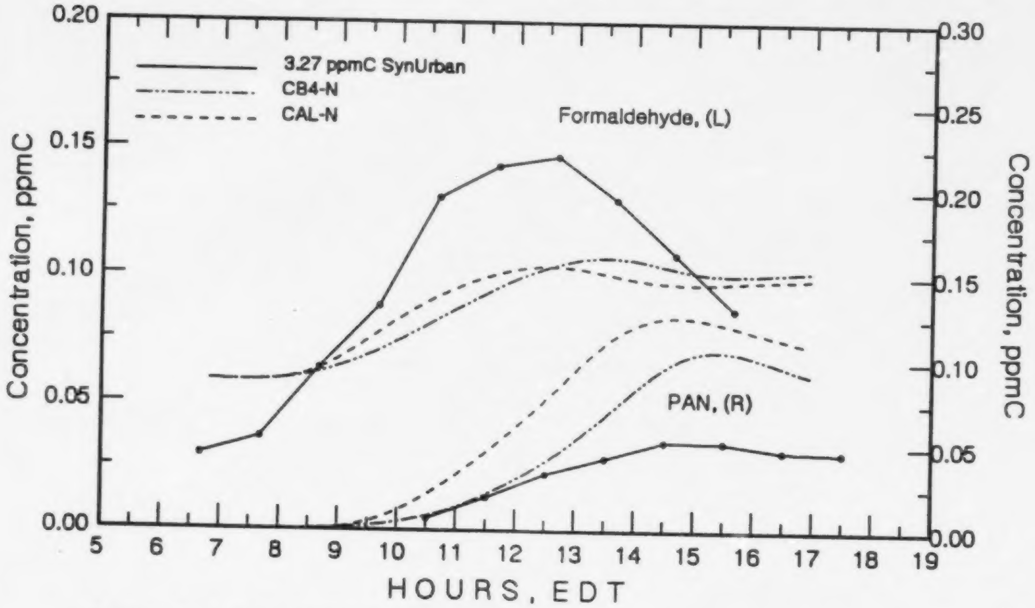


Figure A75. CB4-N and CAL-N Predictions.

September 2, 1984: 1/3 Hydrocarbon Reduction

Top: 1.24 ppmC SynUrban
Bottom: 0.82 ppmC SynUrban

Chamber Observations:

In Figure A76, note the significant decrease in the peak ozone concentration from 0.12 ppm to 0.02 ppm due to the reduction in hydrocarbon.

CB4 and CAL Predictions:

CB4 and CAL predict the NO_x crossover point (Fig A77) adequately on the control side (top), but are considerably early on the reduction side (bottom).

In Figure A78, CB4 and CAL track the observed hydrocarbon decay profiles well.

Nevertheless, both CB4 and CAL over predict the ozone profile (Fig A77) by large margins on both sides of the chamber. The mechanisms also fail to predict the correct relative change in ozone concentrations due to the hydrocarbon reduction.

CB4 and CAL under predict the formaldehyde profiles (Fig. A79) on both sides of the chamber. CB4 under predicts PAN concentrations on the reduction side (bottom) but predicts PAN concentrations correctly on the control side (top). CAL predicts PAN concentrations correctly on the reduction side (bottom) and over predicts PAN concentrations on the control side (top).

CIT Predictions:

In Figure A80, both CIT mechanisms predict the correct NO_x crossover point on the control side (top), but they predict the crossover much earlier than observed on the reduction side (bottom).

The CIT mechanisms predict the ethylene decay profiles correctly in Figure A81.

CIT-1 over predicts the ozone profile (Fig. A80) on both sides of the chamber by the same amount as CAL. CIT-2 correctly predicts the observed ozone profile on the control side, but over predicts the profile observed on the reduction side.

Both CIT mechanisms under predict the formaldehyde and PAN profiles (Fig. A82) observed on both sides of the chamber.

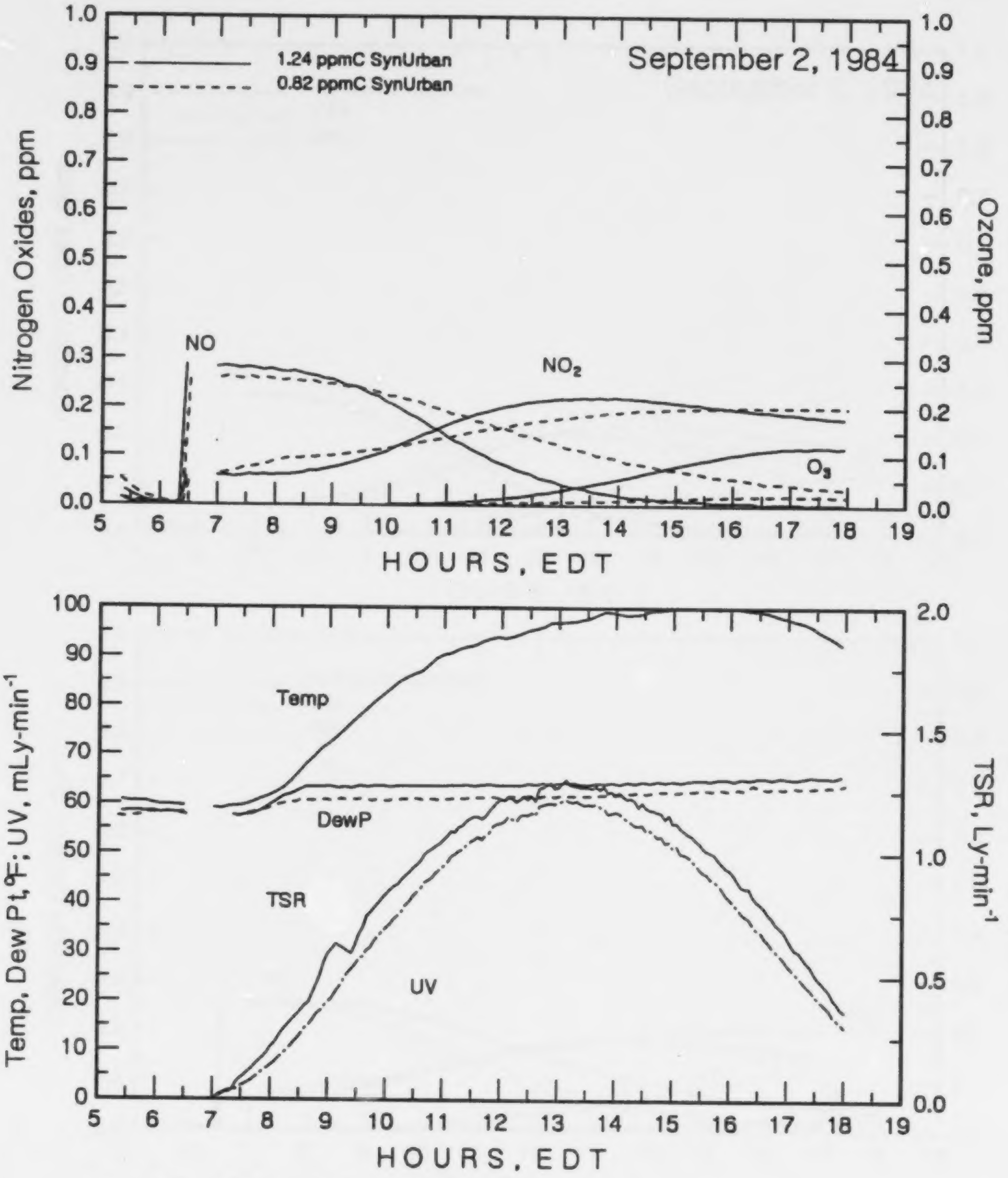
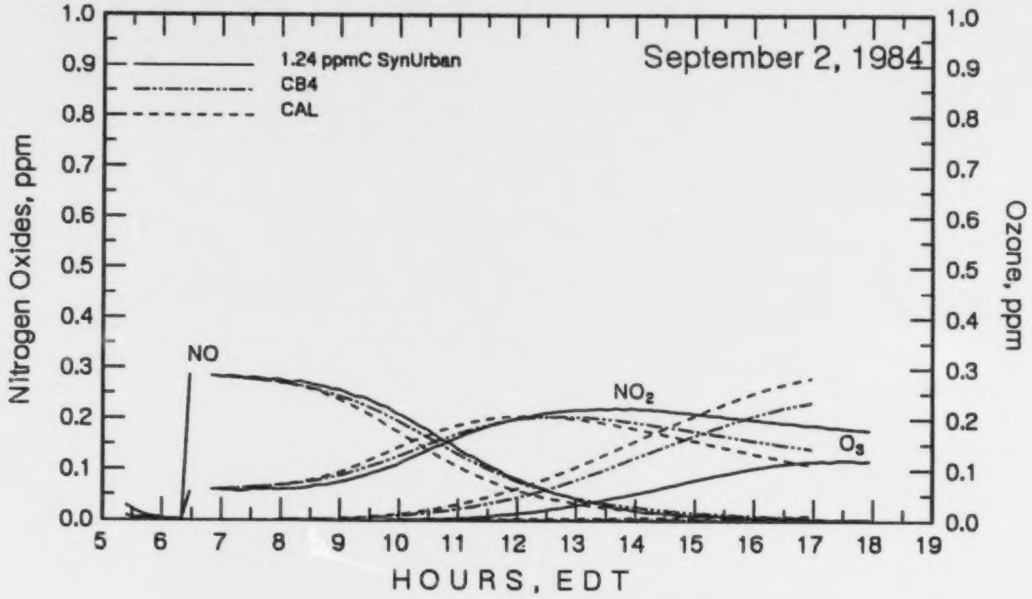


Figure A76. Chamber Observations.



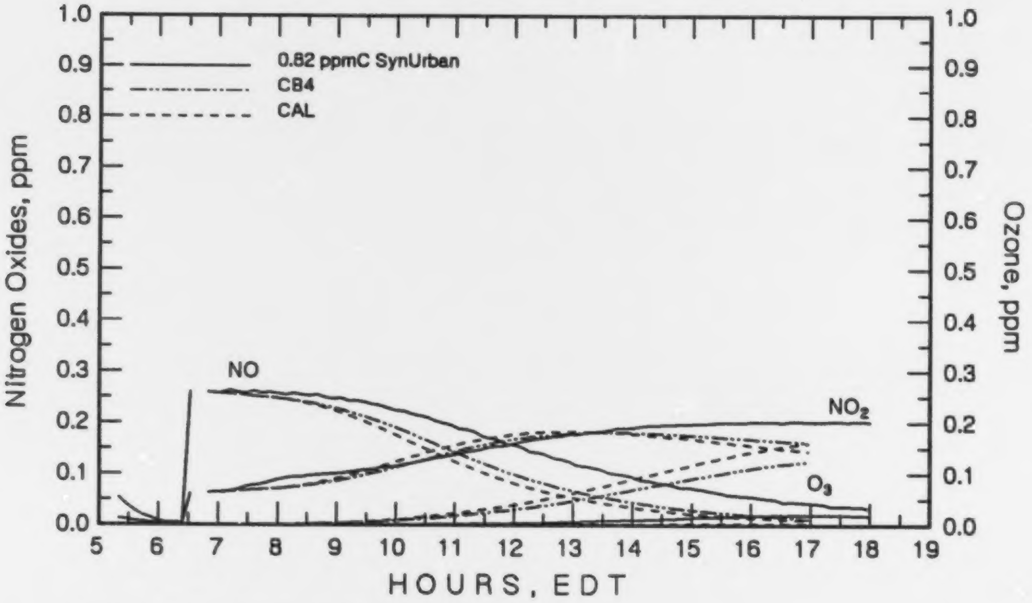
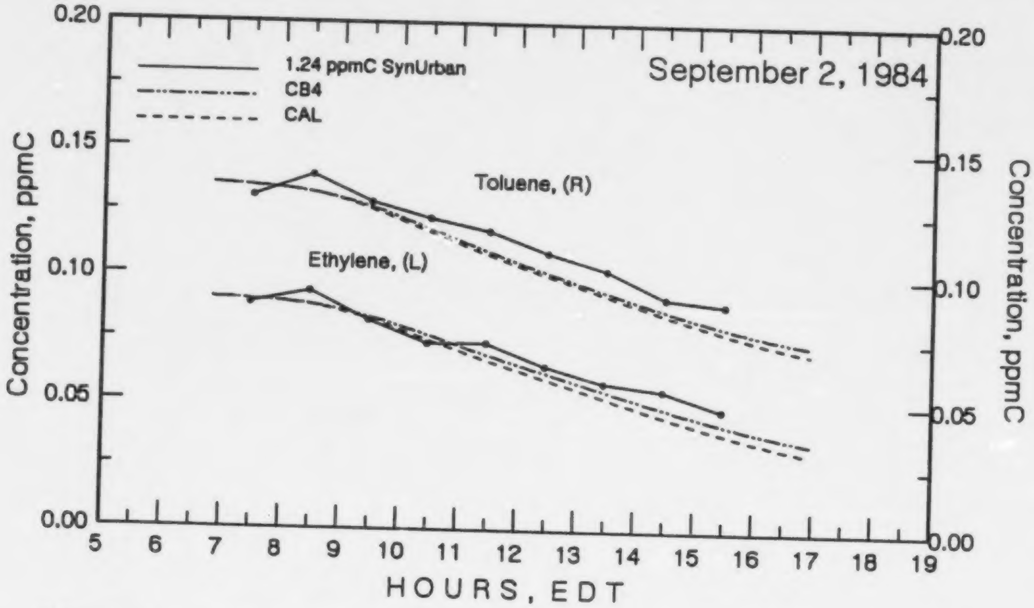


Figure A77. CB4 and CAL Predictions.



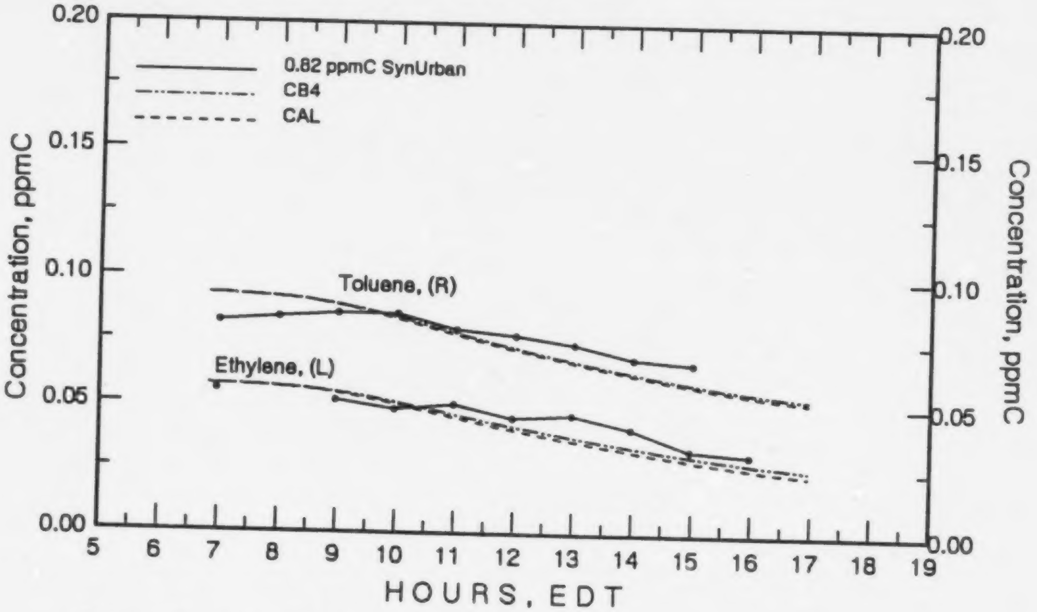


Figure A78. CB4 and CAL Predictions.

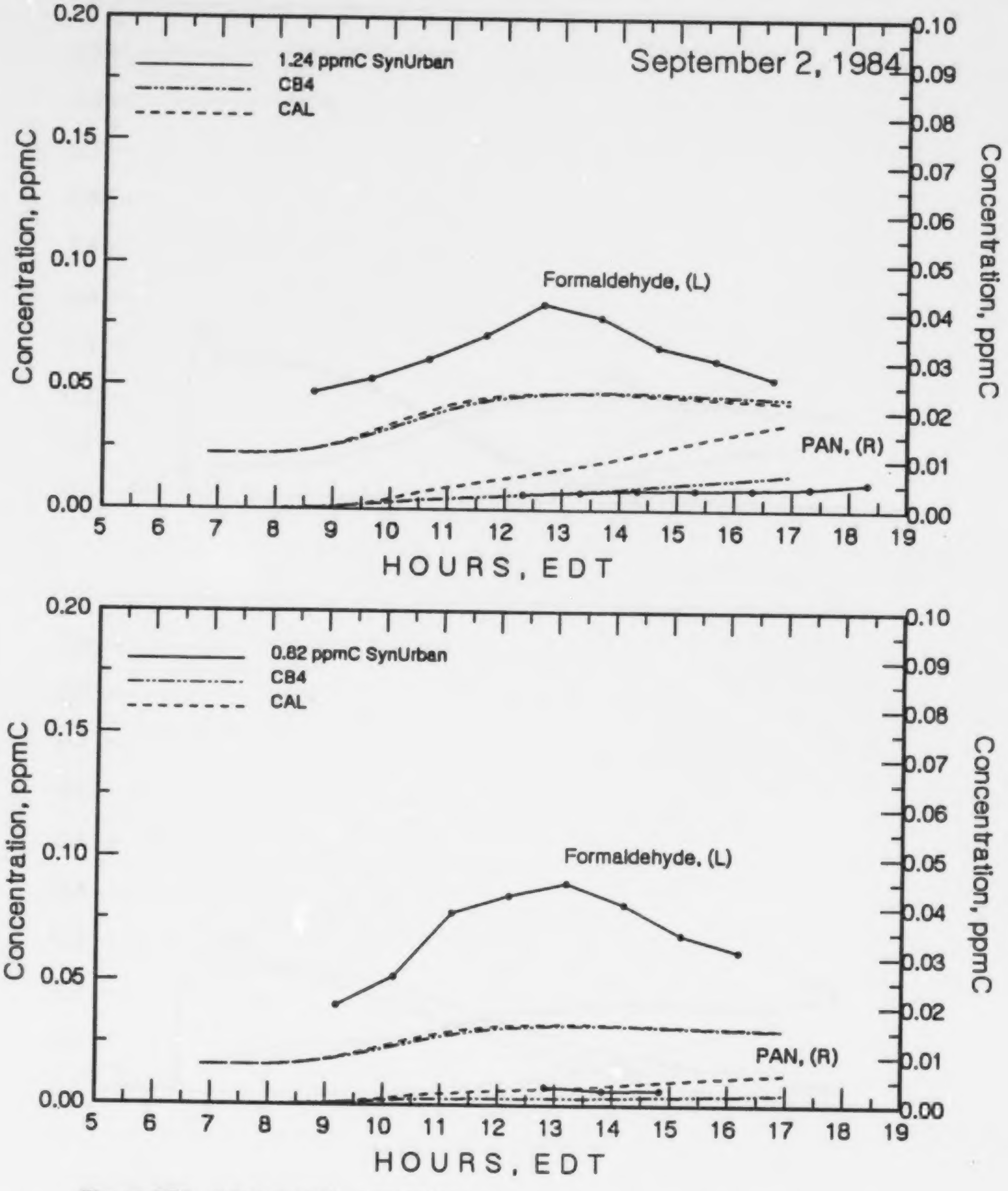


Figure A79. CB4 and CAL Predictions.

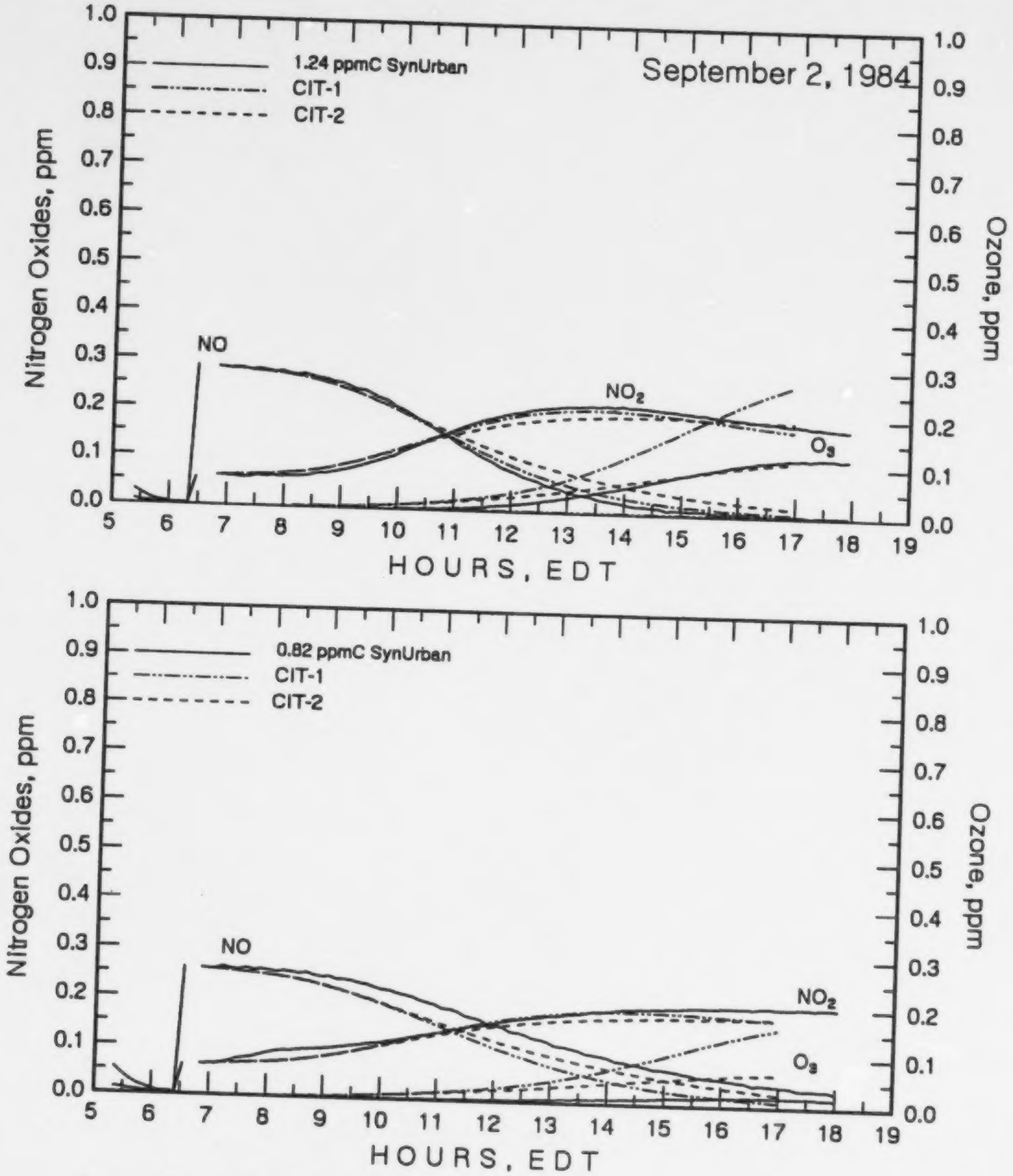
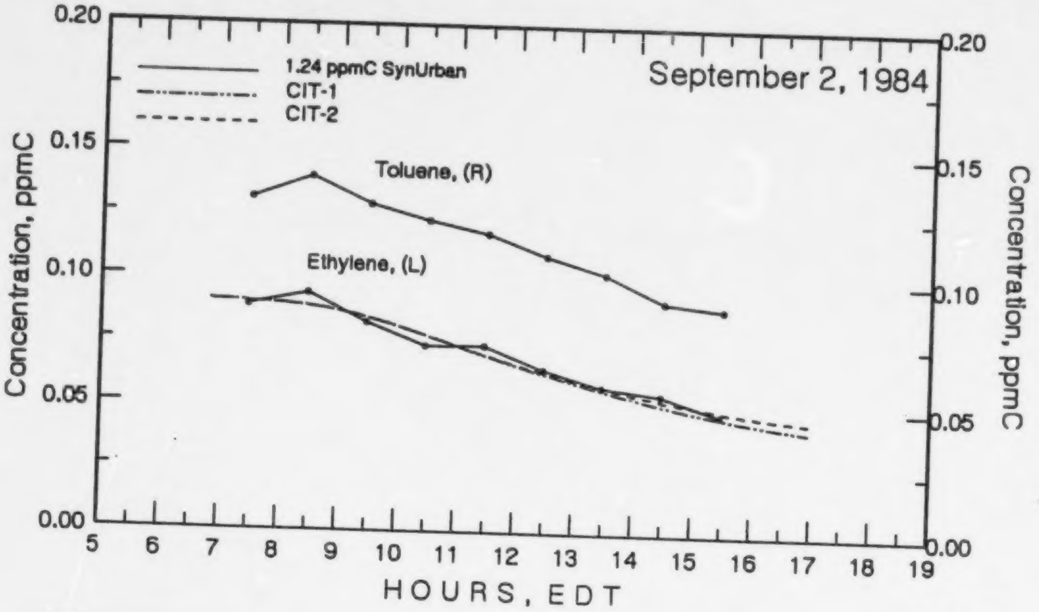


Figure A80. CIT Predictions.



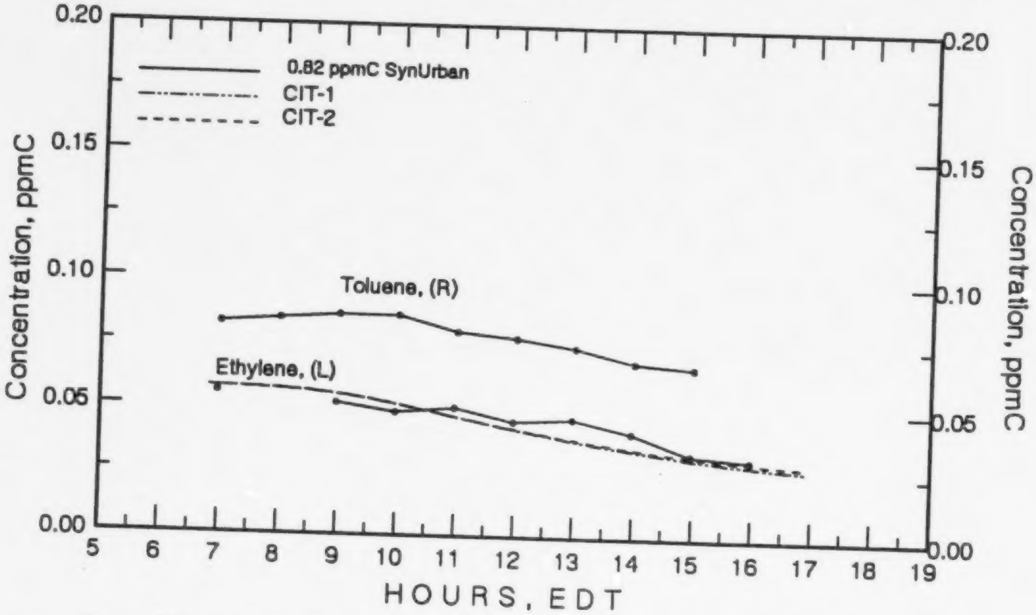


Figure A81. CIT Predictions.

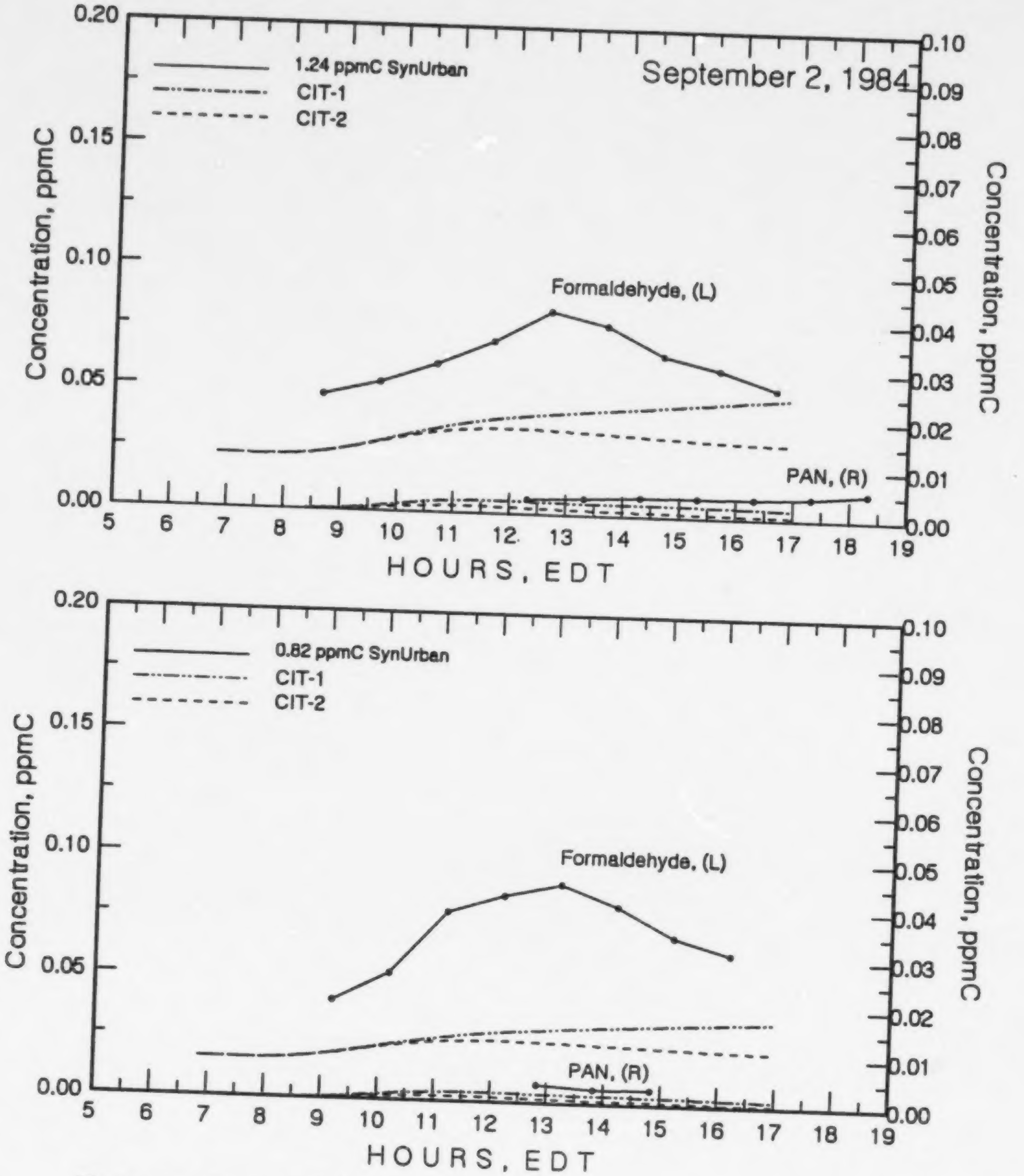


Figure A82. CIT Predictions.

September 3, 1984: 1/3 Methanol Substitution w/20% HCHO

Top: 1.11 ppmC SynUrban
Bottom: 0.79 ppmC SynUrban, 0.3 ppm MEOH, 0.06 ppm HCHO

Chamber Observations:

In Figure A83, there is no effect of the substitution on the concentration of ozone.

CB4 and CAL Predictions:

In Figure A84, CB4 and CAL predict NO_x crossover points which are earlier than the observed point.

CB4 and CAL predict faster hydrocarbon decays (Fig. A85) on the control side (top) than were observed, but the predicted decay profiles on the substitution side (bottom) appear adequate.

Both CB4 and CAL significantly over predict the concentration of ozone produced (Fig. A84) on both sides of the chamber. However, the mechanisms correctly predict that the substitution has no effect on the observed ozone concentrations.

The formaldehyde concentration profile (Fig. A86) is tracked well by both CB4 and CAL on both sides of the chamber. There are no PAN observations for this day to compare to the model predictions.

CIT Predictions:

The CIT mechanisms adequately predict the NO_x crossover point (Fig. A87) and the ethylene decay profile (Fig. A88) on both sides of the chamber.

CIT-1 over predicts the ozone concentration profile (Fig. A87) on both sides of the chamber by the same significant margin as CB4 and CAL. CIT-2 also over predicts the ozone concentration profile but not by as much as the other mechanisms.

The formaldehyde concentration profile (Fig. A89) generated by CIT-1 is similar to those generated by CB4 and CAL. It tracks the observed profile well until the afternoon when it under predicts the observed concentrations. CIT-2 shows the same under predicts of afternoon formaldehyde concentrations but to a greater extent.

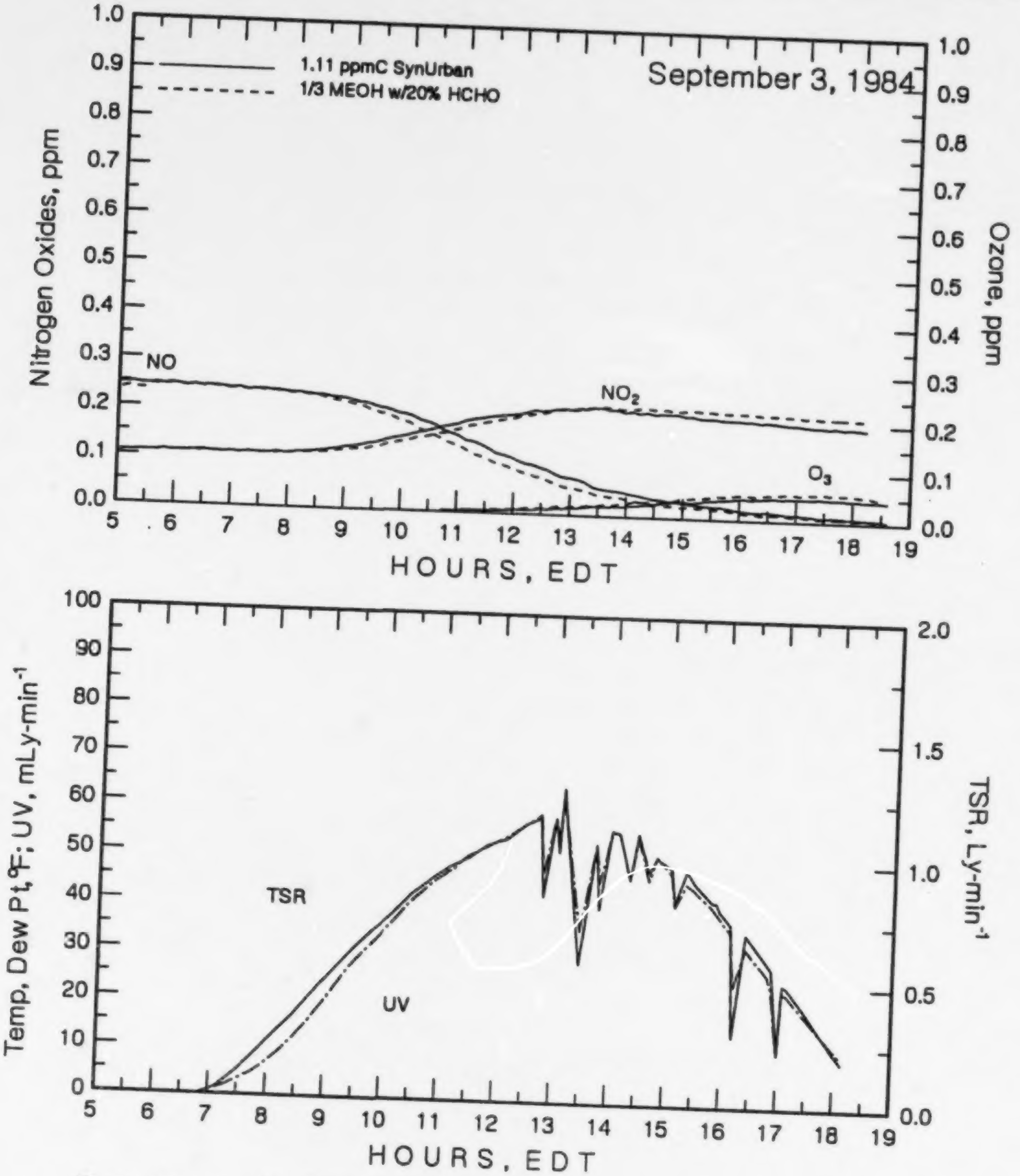
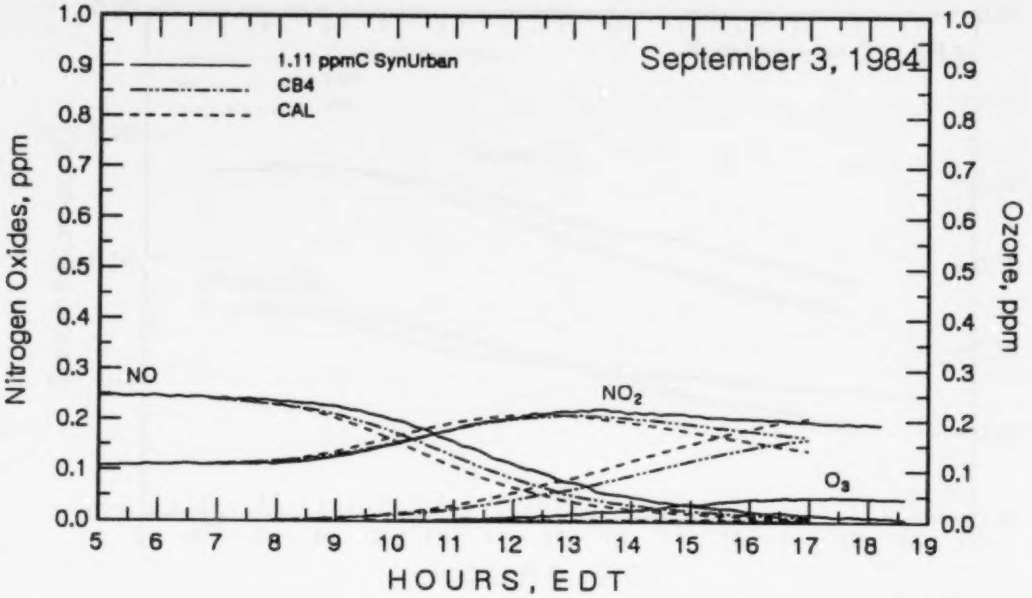


Figure A83. Chamber Observations.



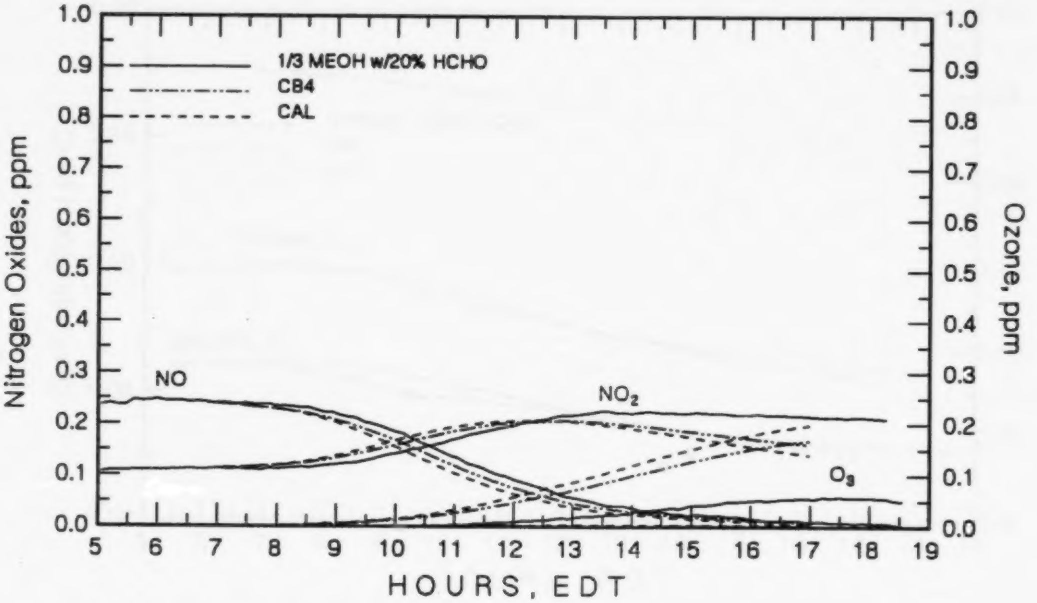


Figure A84. CB4 and CAL Predictions.

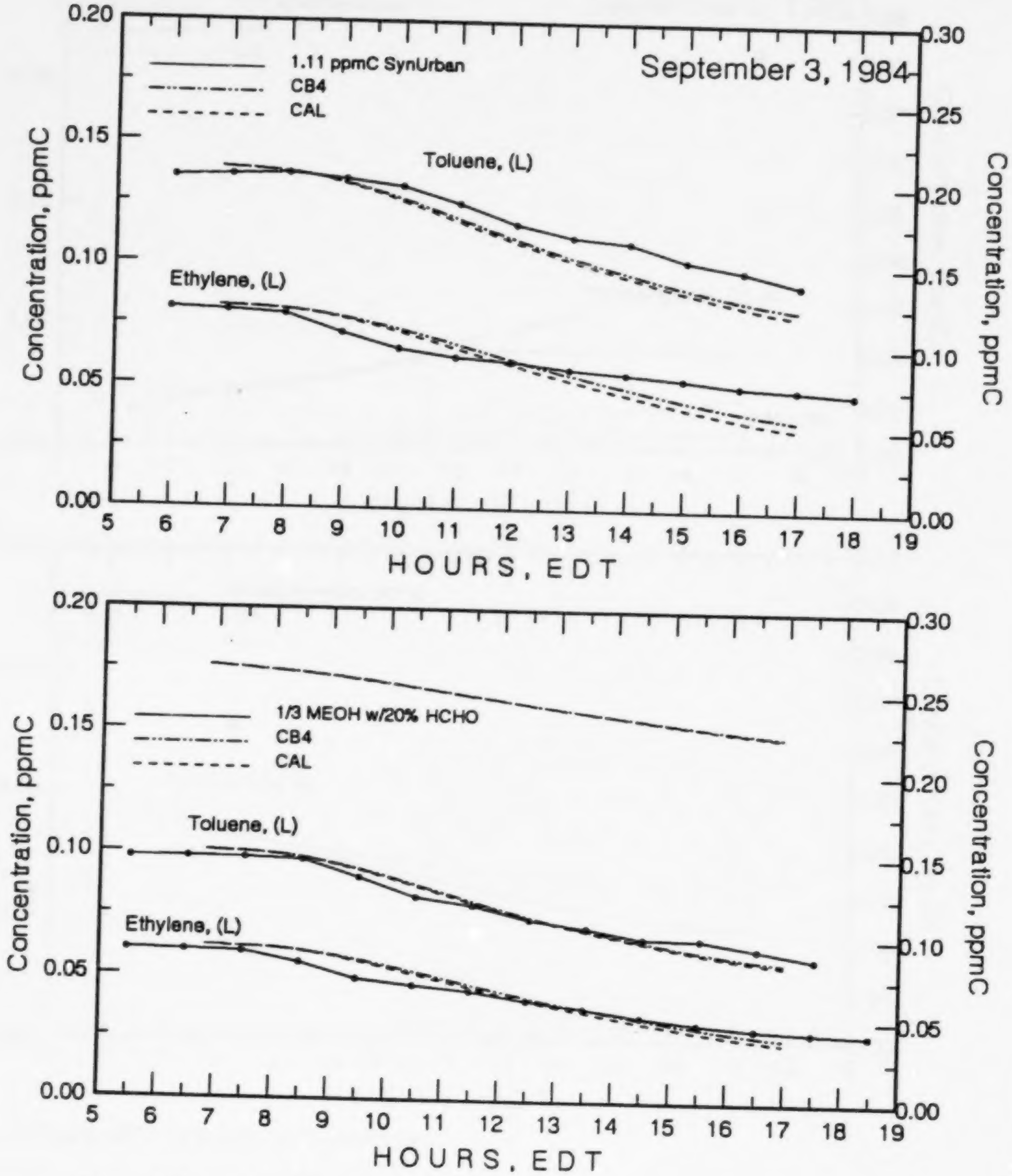
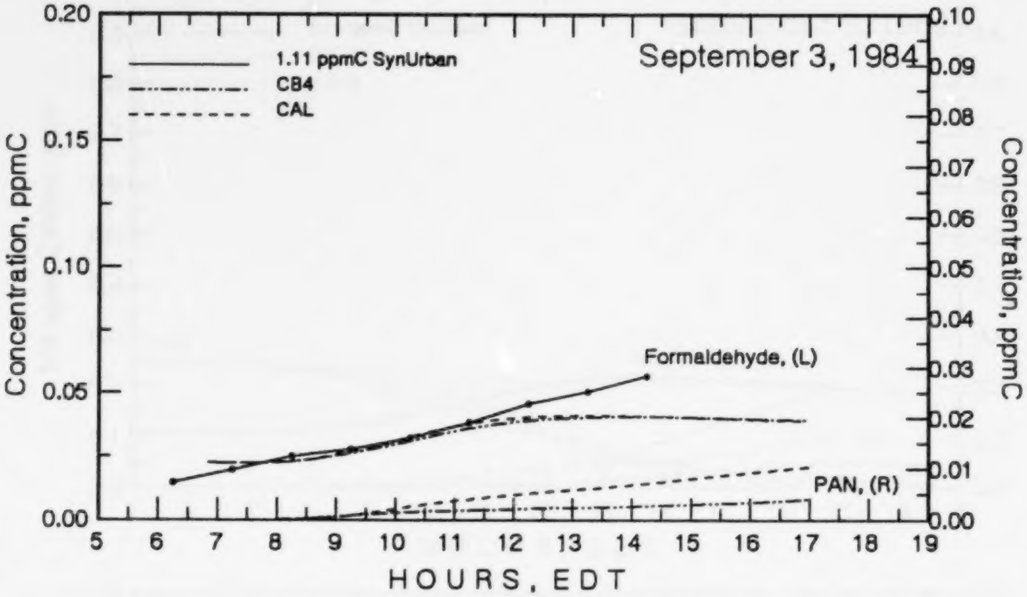


Figure A85. CB4 and CAL Predictions.



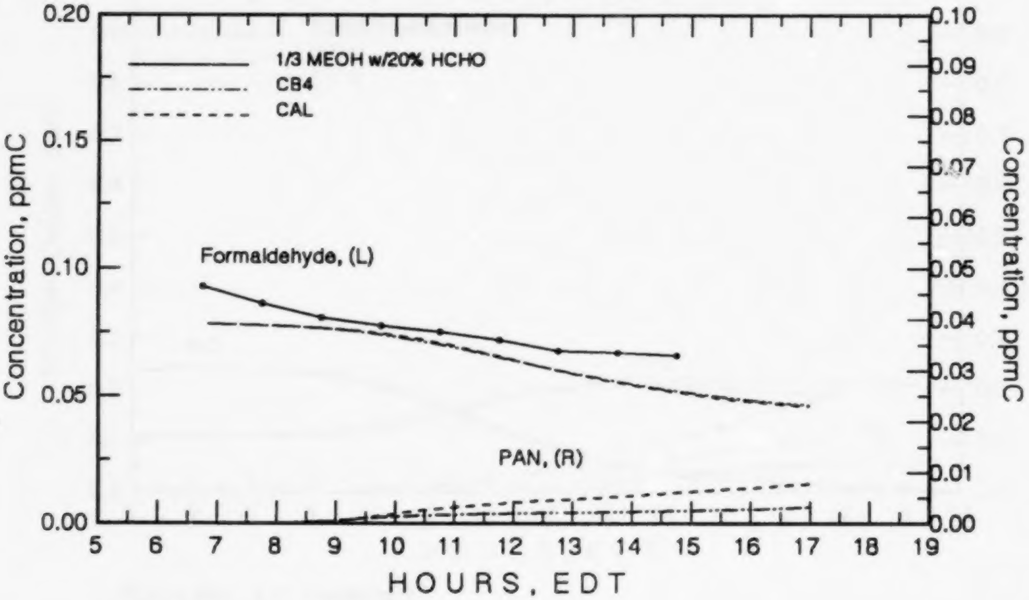
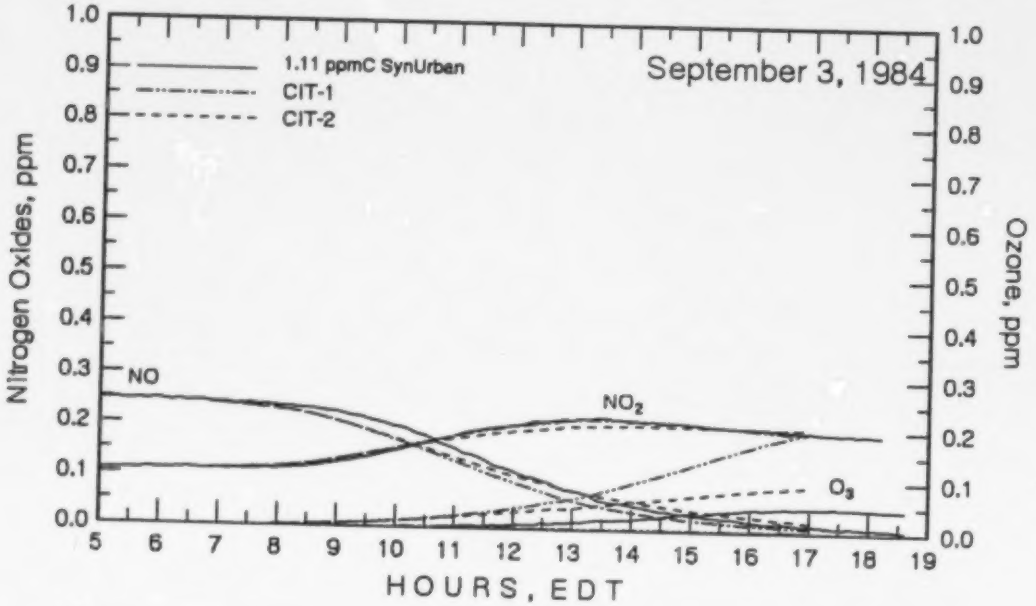


Figure A86. CB4 and CAL Predictions.



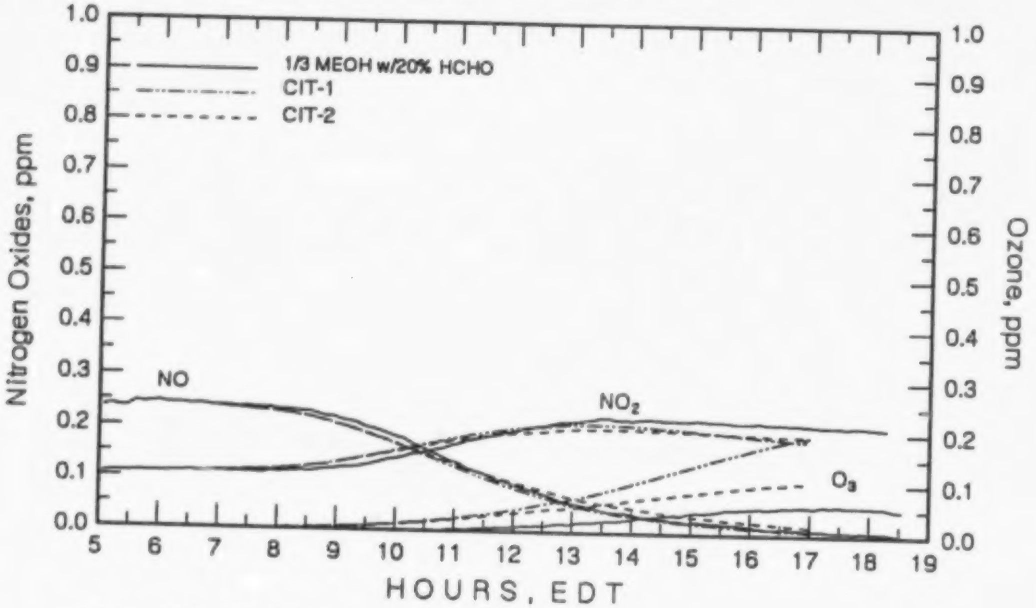


Figure A87. CIT Predictions.

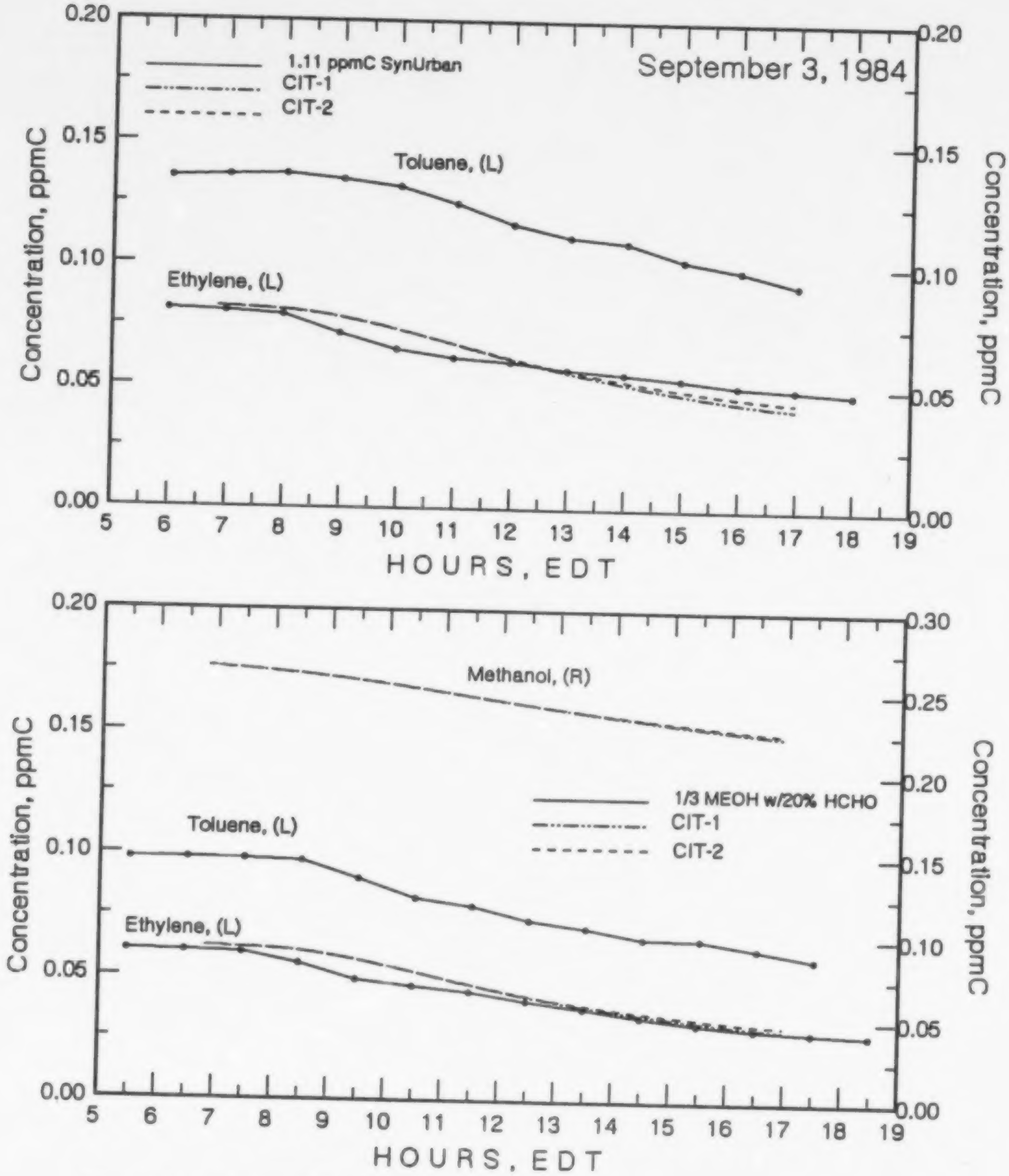
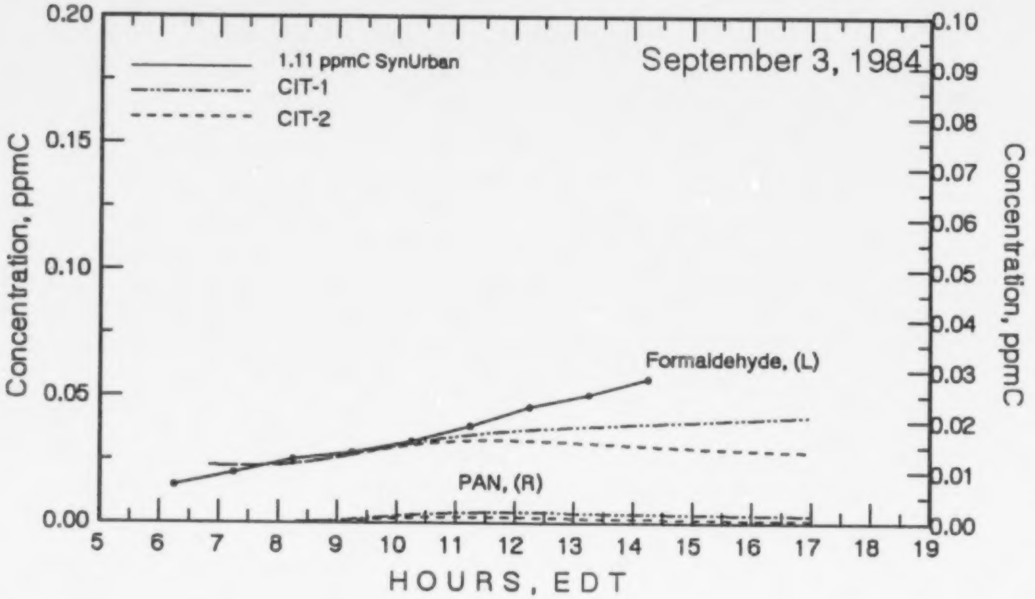


Figure A88. CIT Predictions.



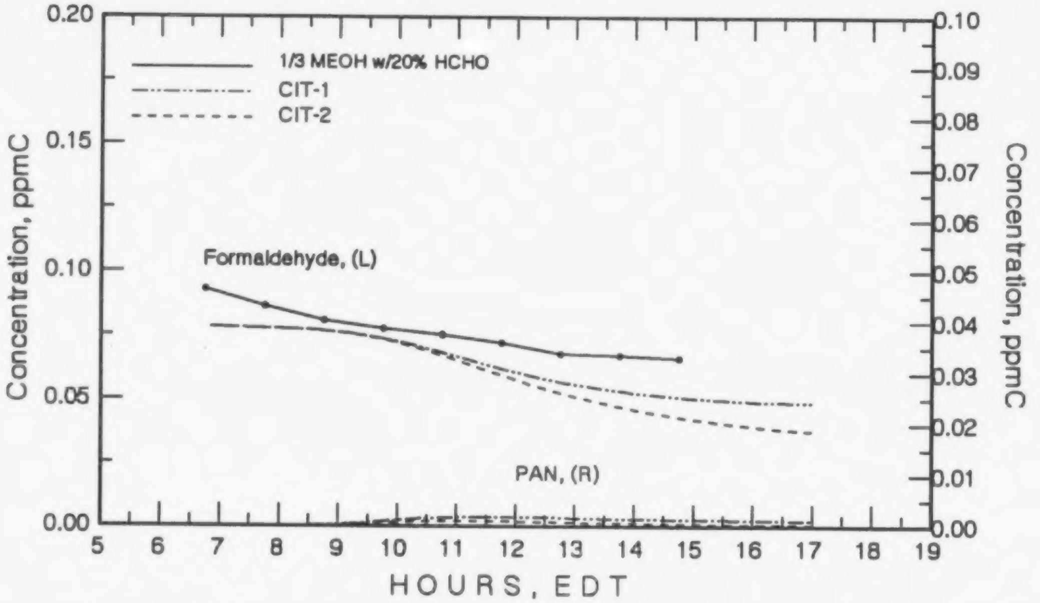


Figure A89. CIT Predictions.

September 8, 1984: 1/3 Hydrocarbon Reduction

Top: 1.92 ppmC SynAutoUrb
Bottom: 2.84 ppmC SynAutoUrb

Chamber Observations:

The effect of the hydrocarbon reduction was to lower and delay the peak ozone concentration (Fig. A90).

CB4 and CAL Predictions:

The NO_x crossover points (Fig. A91) predicted by CB4 and CAL are about a half hour earlier than was observed on either side of the chamber.

The ethylene decay profiles (Fig. A92) predicted by CB4 and CAL are too fast throughout the day on the reduction side (top) and in the afternoon on the control side (bottom). The predicted toluene decay profiles are adequate on both sides of the chamber.

CB4 and CAL over predict the peak ozone concentration (Fig. A91) on the reduction side. Although the mechanisms also over predict the ozone concentration profile on the control side, the P/O ratios are less than 1.2. CB4 and CAL under predict the relative change in the peak ozone concentration due to the reduction.

There are no formaldehyde observations for this experiment to compare to the model predictions. The predicted PAN concentrations (Fig. A93) generated by CB4 and CAL are much greater than the observed concentrations.

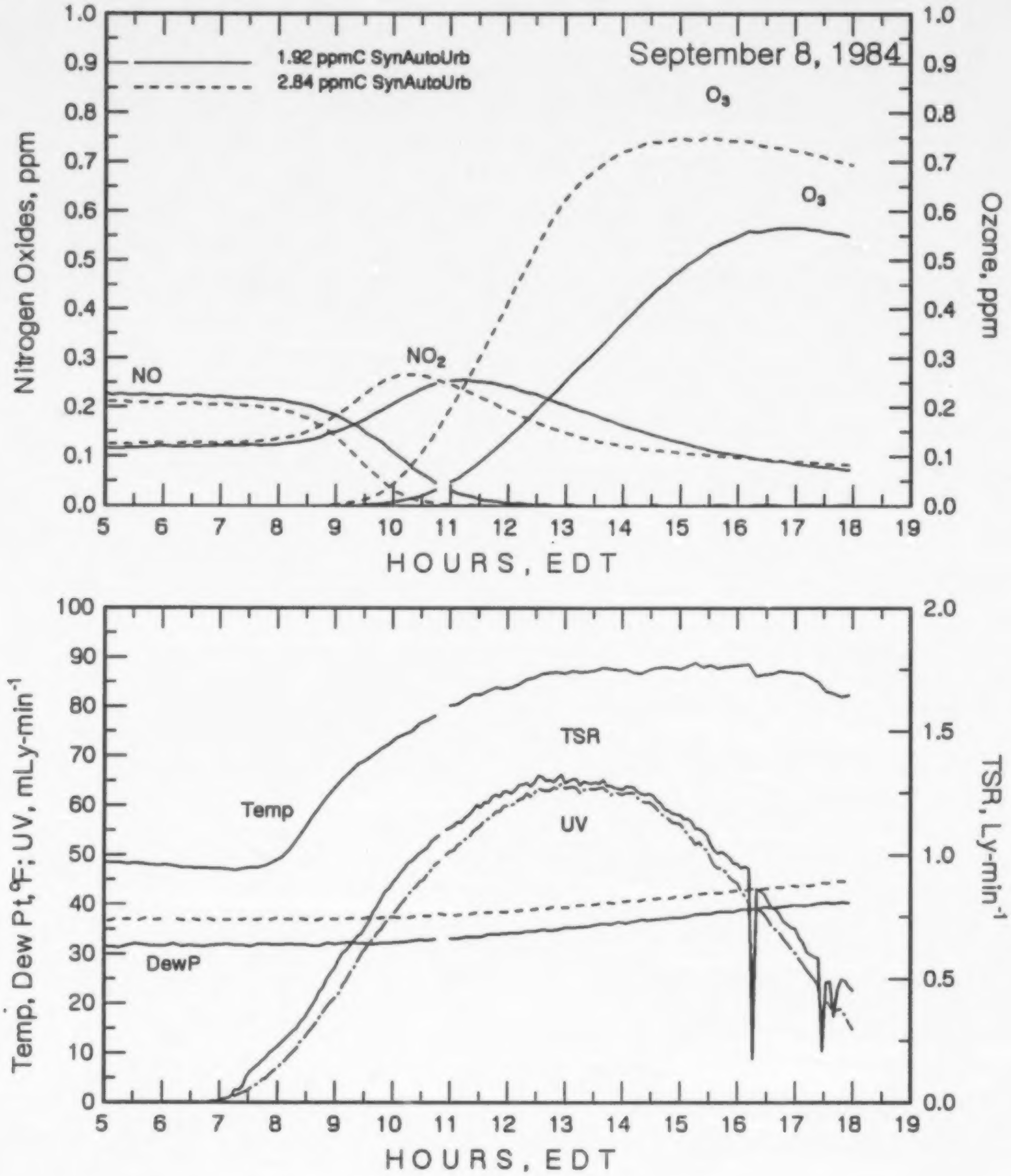


Figure A90. Chamber Observations.

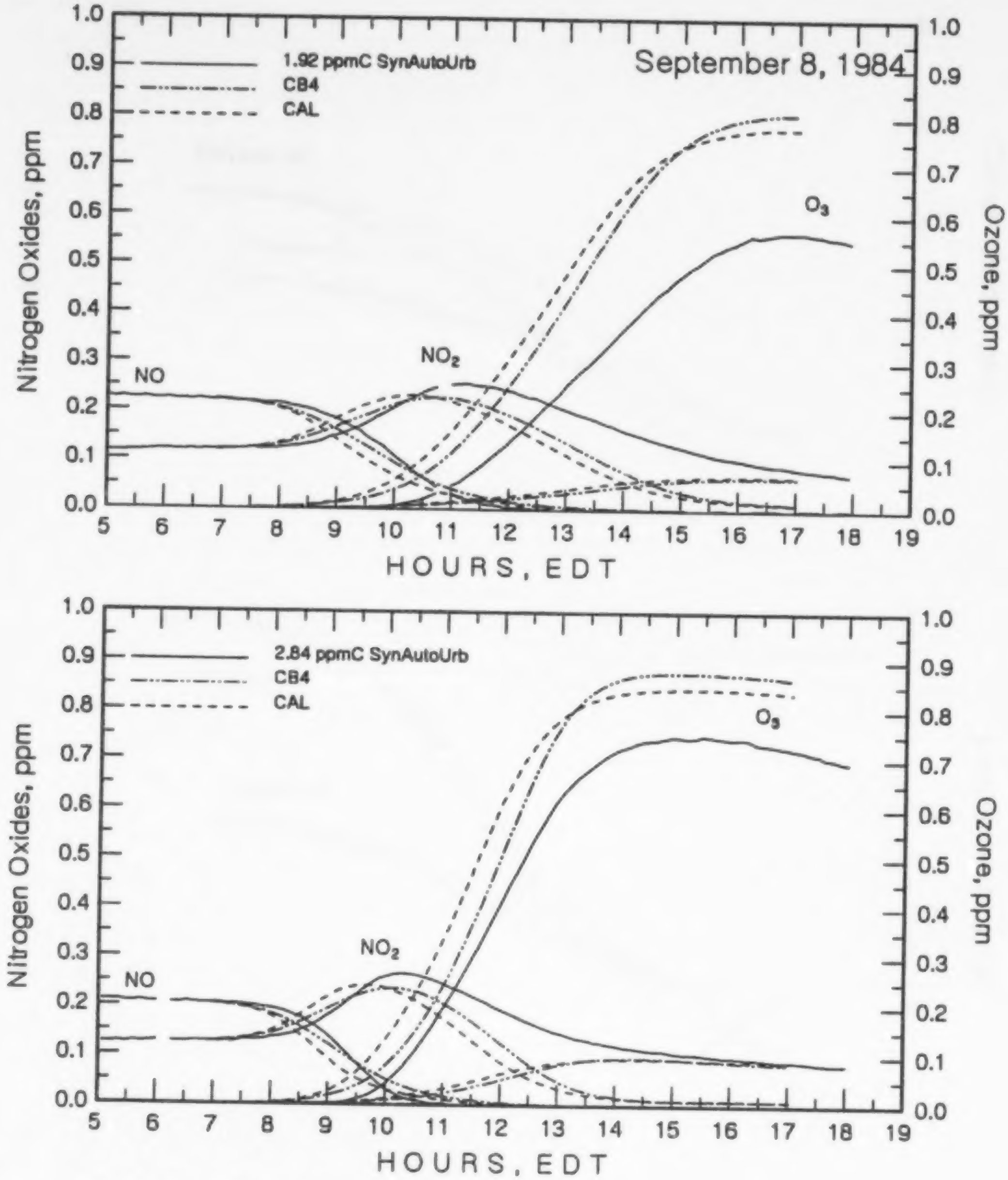


Figure A91. CB4 and CAL Predictions.

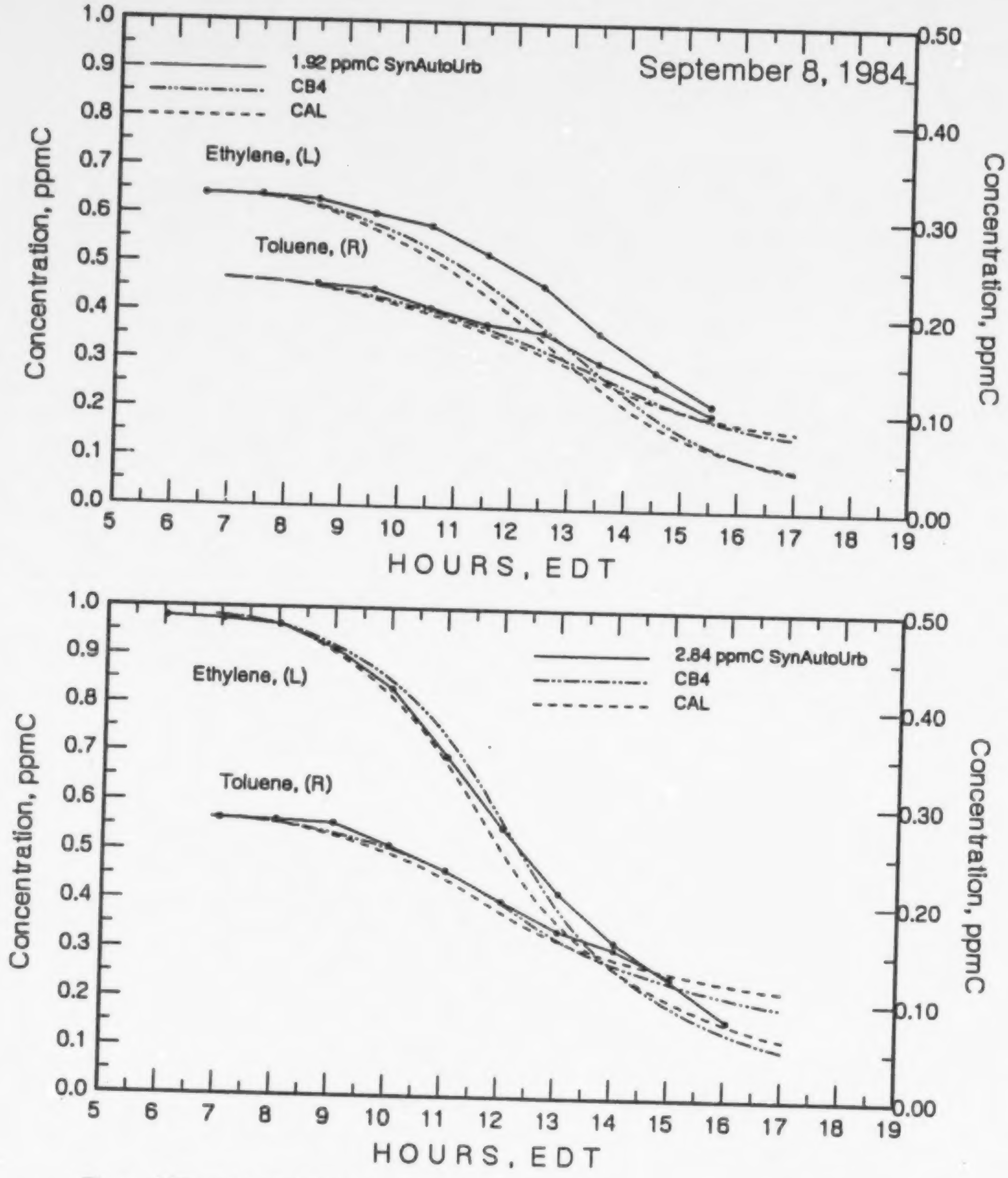


Figure A92. CB4 and CAL Predictions.

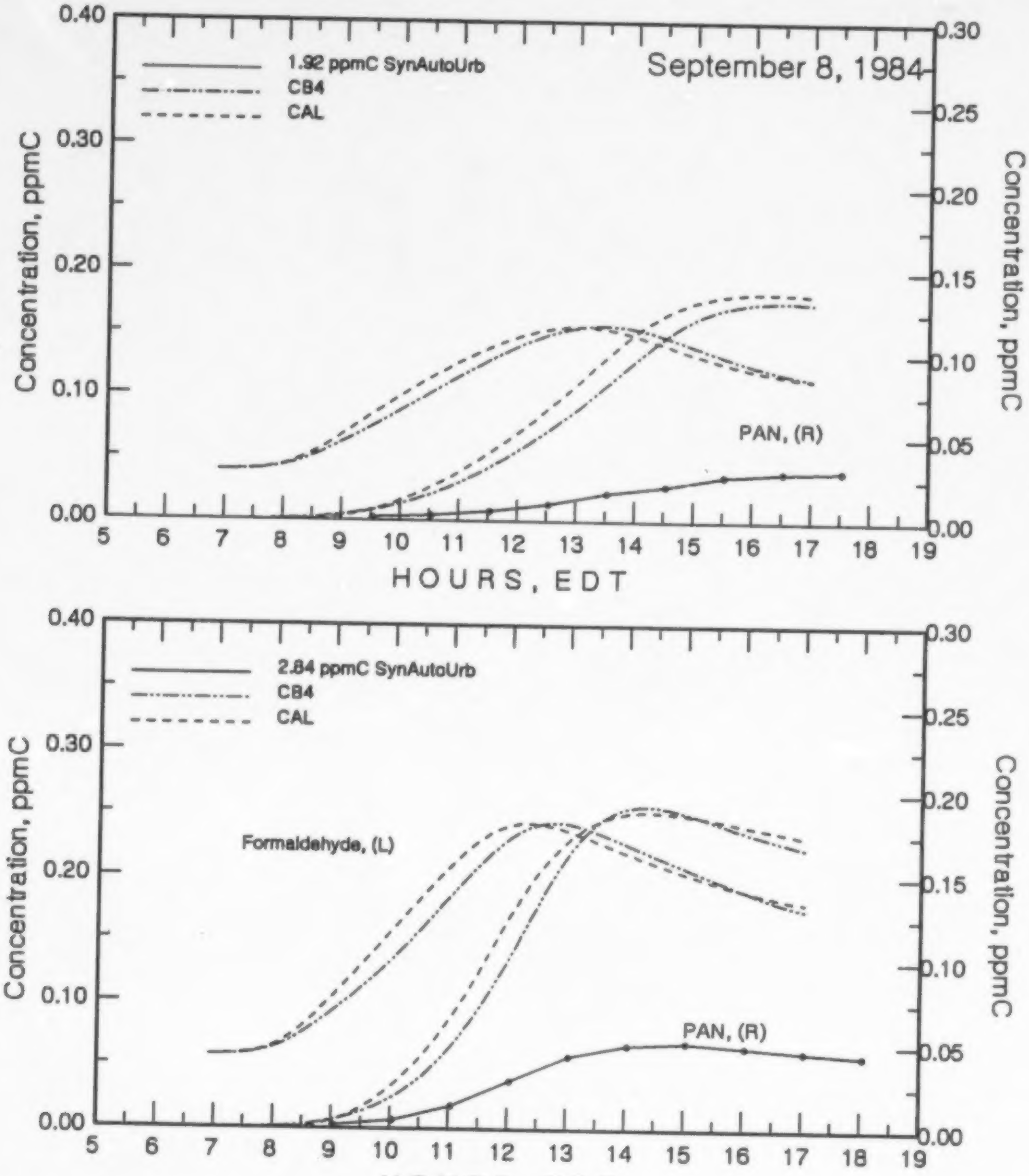


Figure A93. CB4 and CAL Predictions.

September 17, 1984: 1/3 Methanol Substitution w/10% HCHO

Top: 2.22 ppmC SynAutoUrb
Bottom: 1.45 ppmC SynAutoUrb, 0.6 ppm MEOH, 0.08 ppm HCHO

Chamber Observations:

In Figure A94, the temperature is at or below the dew point during the morning. This suggests that condensation may have formed on the chamber walls. The effect of the substitution is to delay and lower the peak ozone concentration.

CB4 and CAL Predictions:

The NO_x crossover points (Fig. A95) predicted by CB4 and CAL occur earlier than the observed crossover points on both sides of the chamber.

The toluene and methanol decay profiles (Fig. A96) are predicted well by CB4 and CAL on both sides of the chamber. There is a discrepancy between the reported initial concentration of ethylene and the concentrations in the Seg file. The initial concentration is derived from an analysis of the injected hydrocarbon mixture and is probably more accurate than the Seg file data which may have been processed with an incorrect calibration factor.

The ozone concentration profile (Fig. A95) is over predicted by CB4 and CAL on both sides of the chamber, but the P/O ratios are less than 1.3.

CB4 and CAL under predict the peak formaldehyde concentration (Fig. A97) on the control side (top). Although the mechanisms also under predict the formaldehyde peak on the substitution side (bottom), the P/O ratios are less than 1.3. The PAN concentration profile is grossly over estimated by CB4 and CAL on both sides of the chamber.

Wall Model Effects:

Switching to Killus's wall model (Figs. A98-100) improves the overall performance of CB4 and CAL. Eliminating the wall reactions (Figs. A101-3) further improves the performance of CB4 and CAL with regards to ozone and PAN but degrades their performance with regards to formaldehyde and hydrocarbon decay.

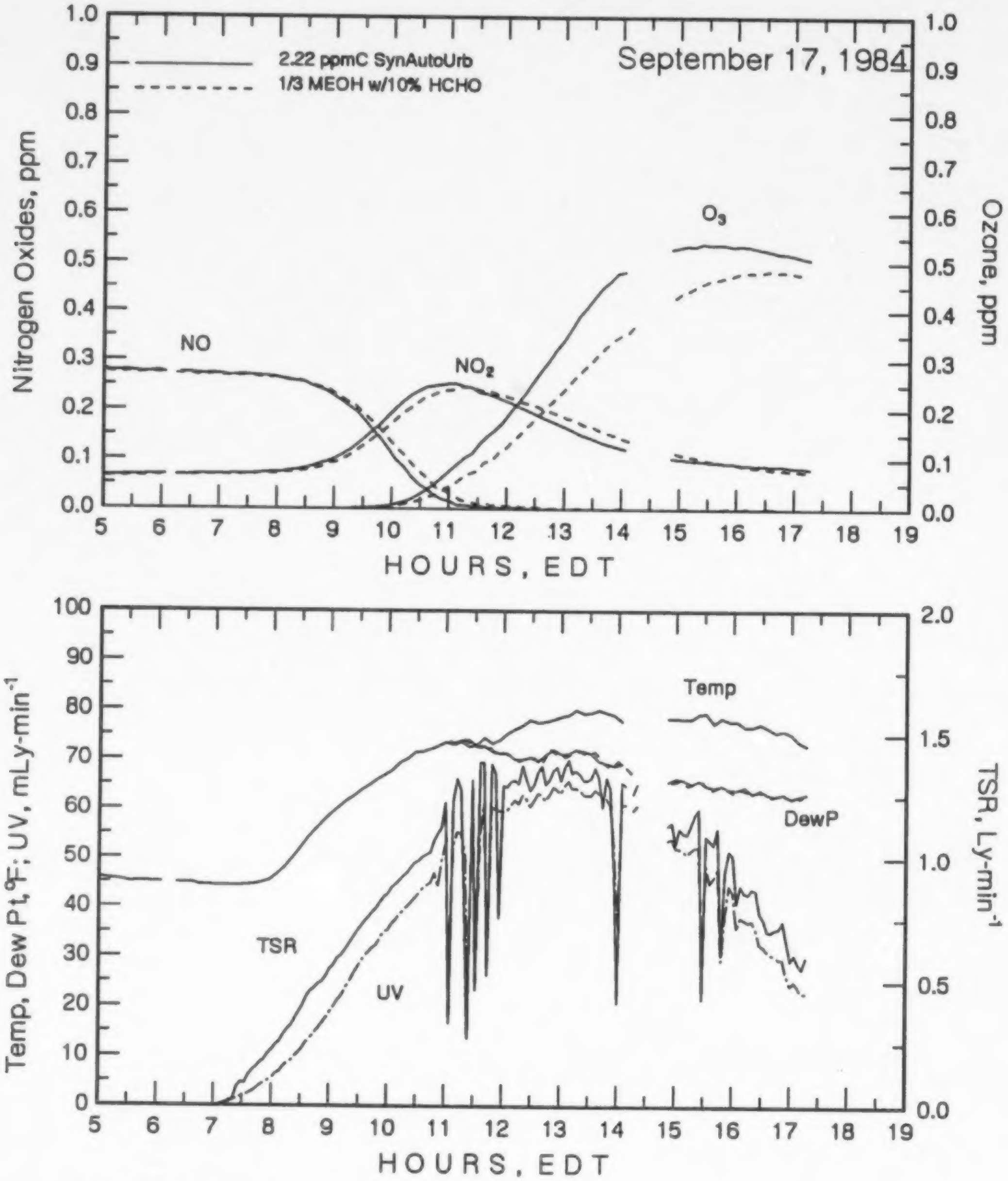


Figure A94. Chamber Observations.

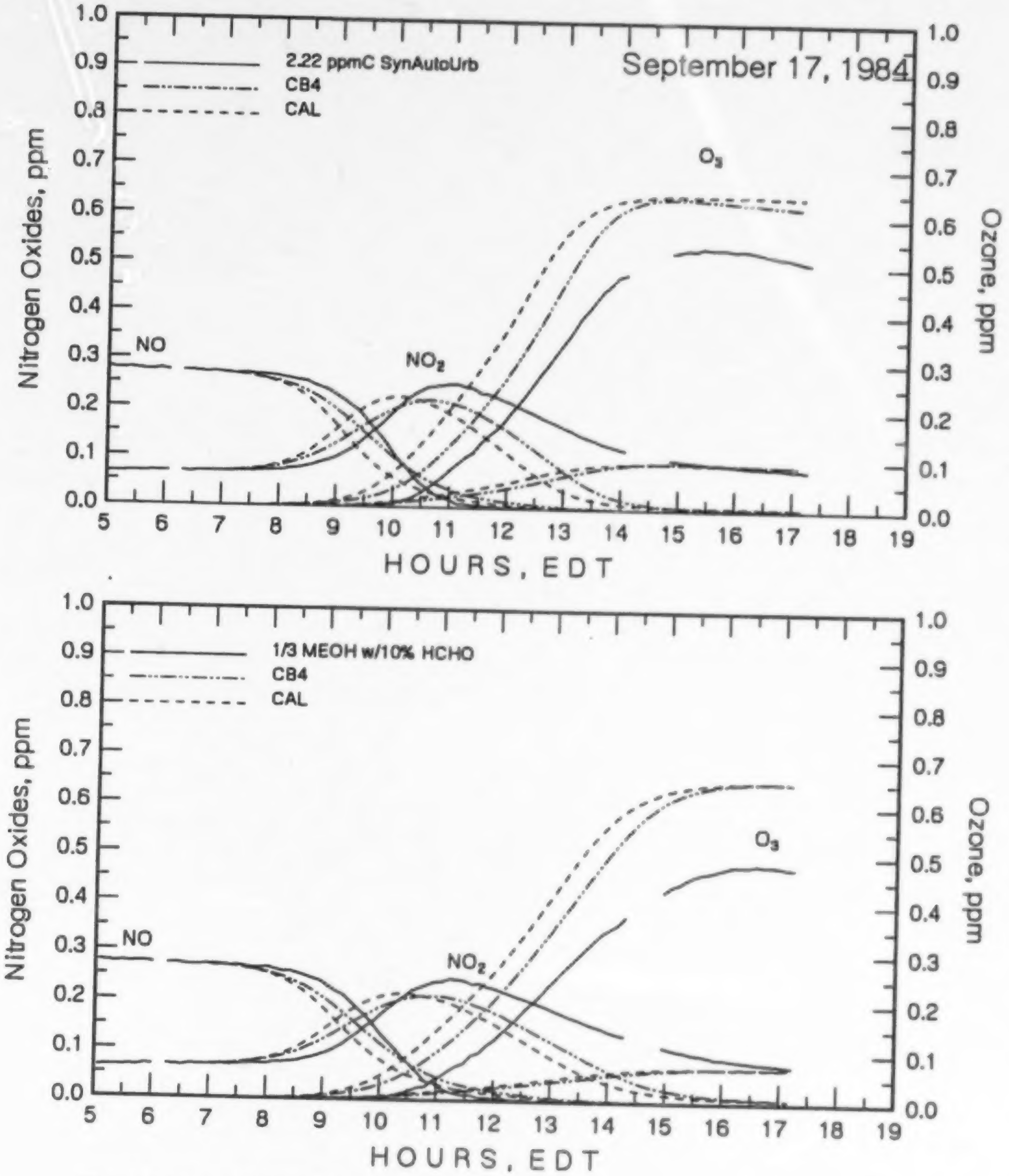
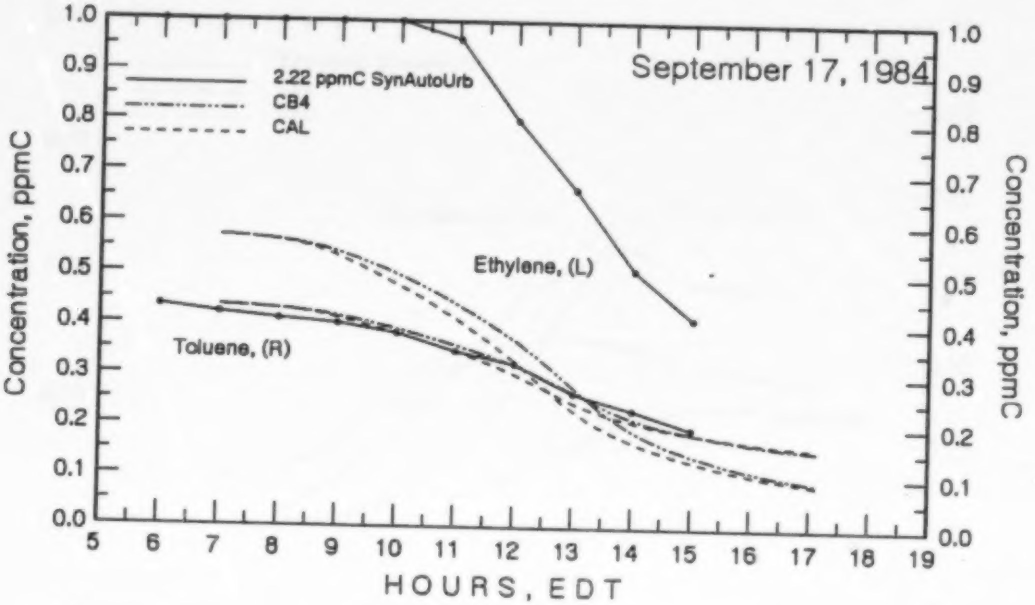


Figure A95. CB4 and CAL Predictions.



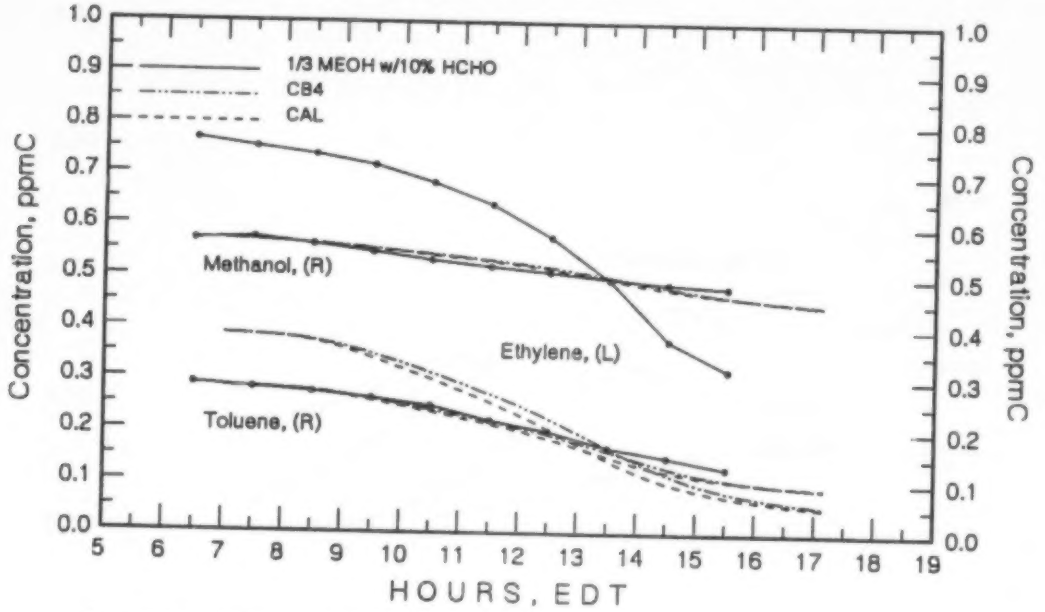


Figure A96. CB4 and CAL Predictions.

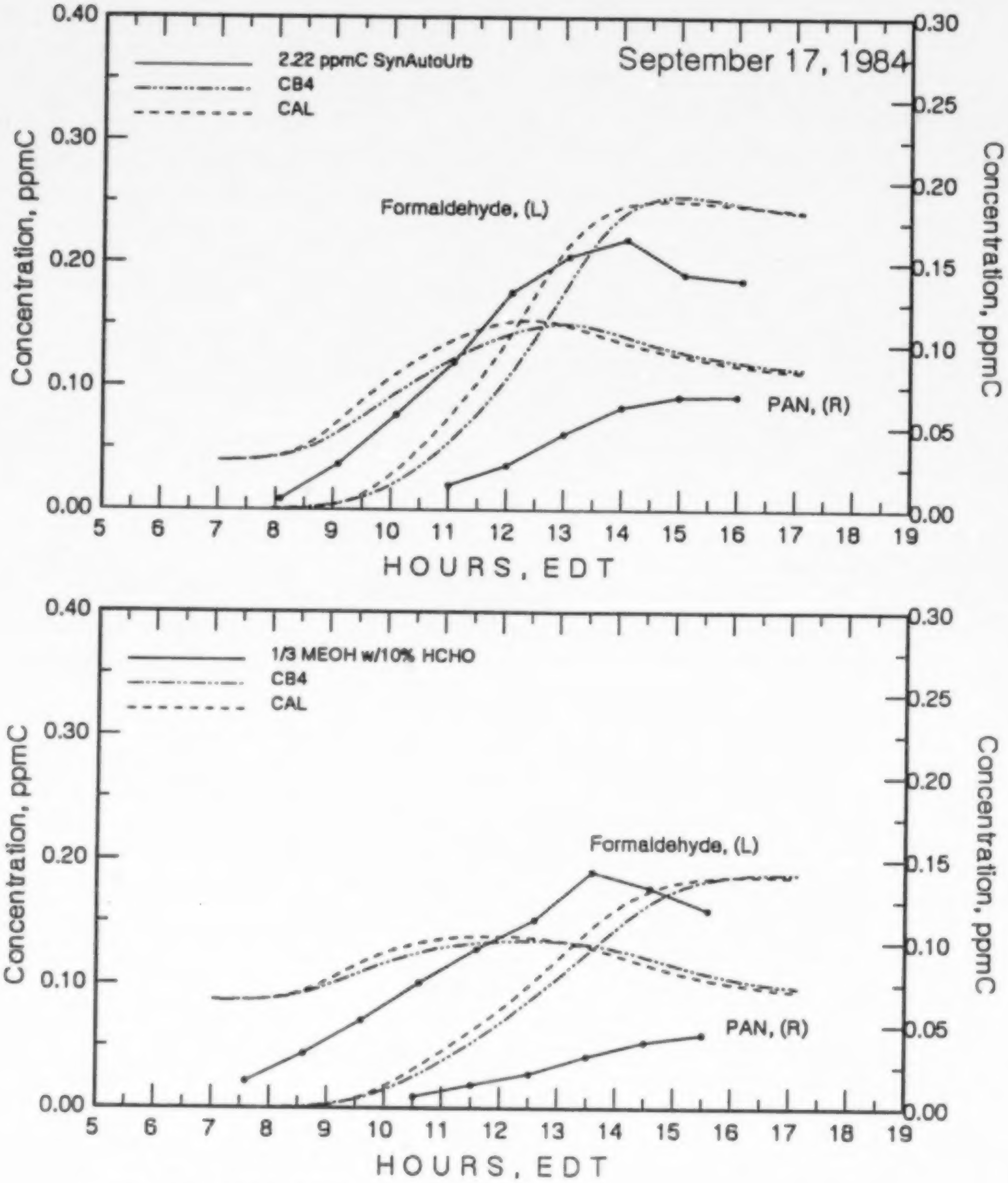


Figure A97. CB4 and CAL Predictions.

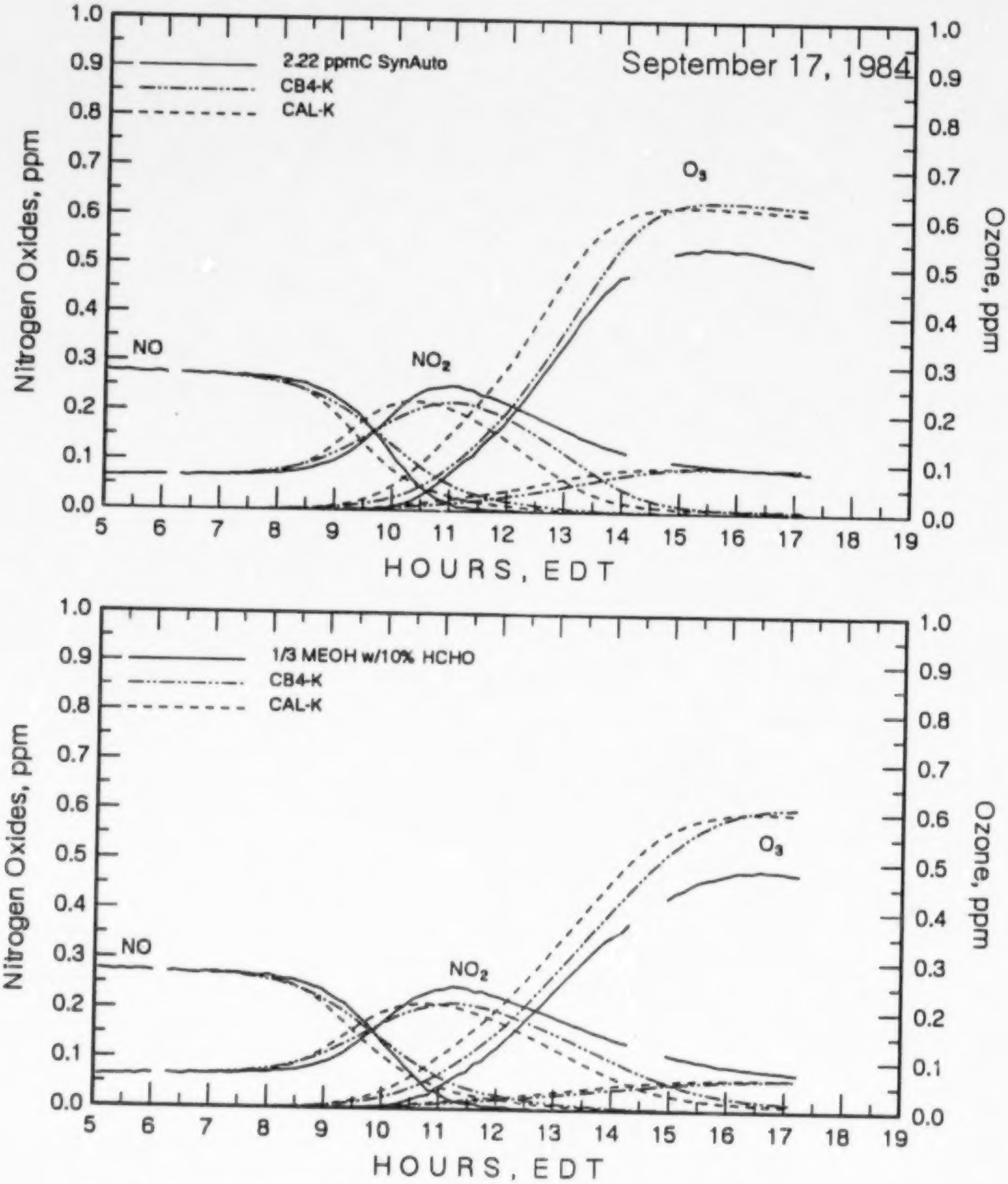


Figure A98. CB4-K and CAL-K Predictions.

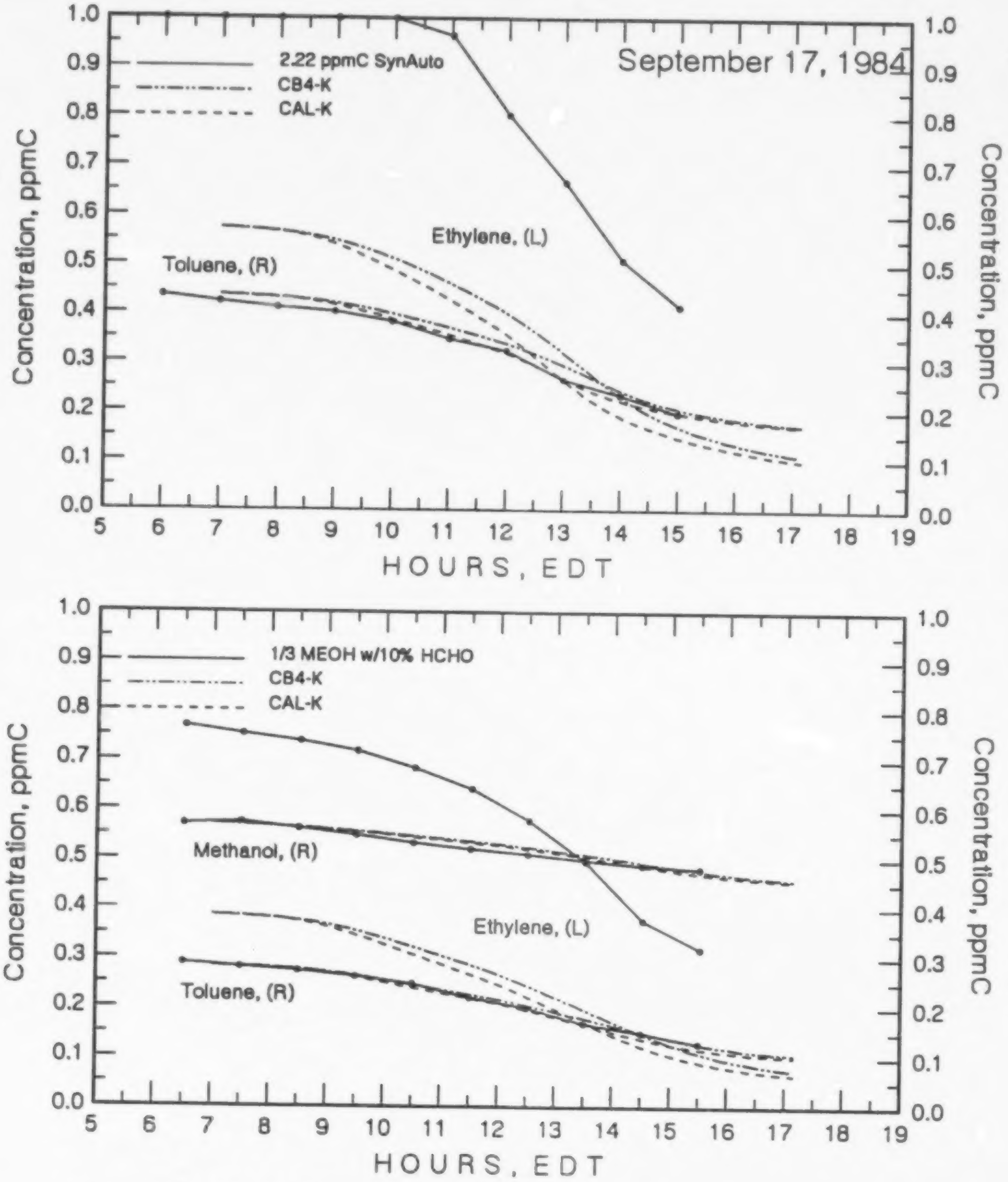
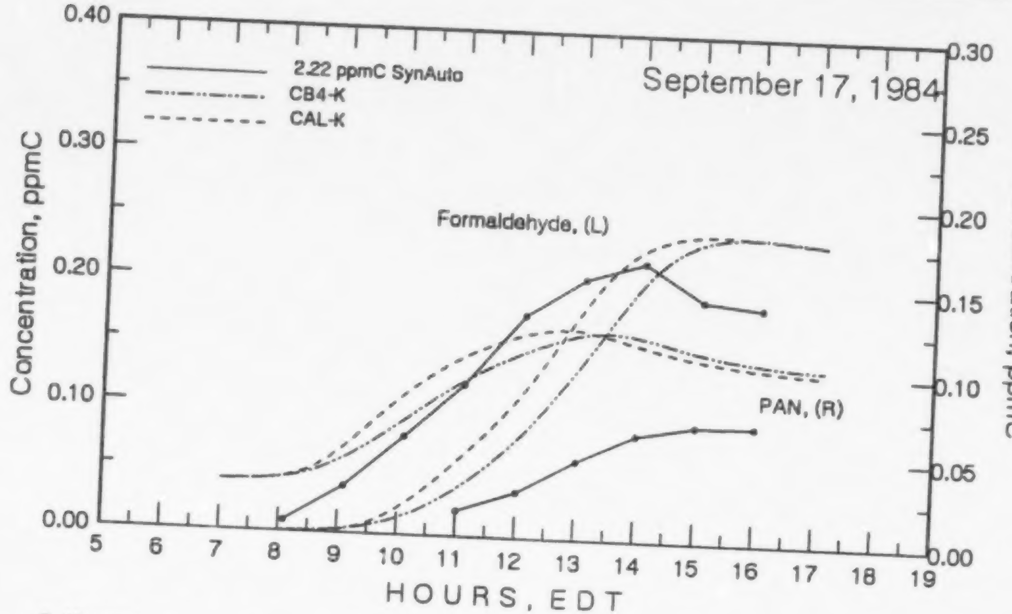


Figure A99. CB4-K and CAL-K Predictions.



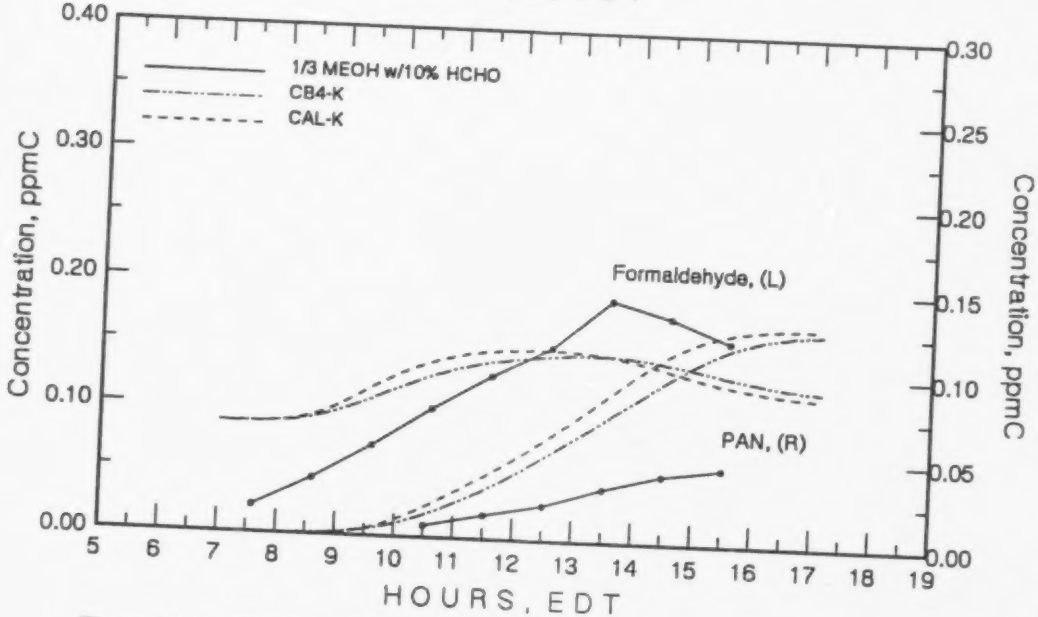
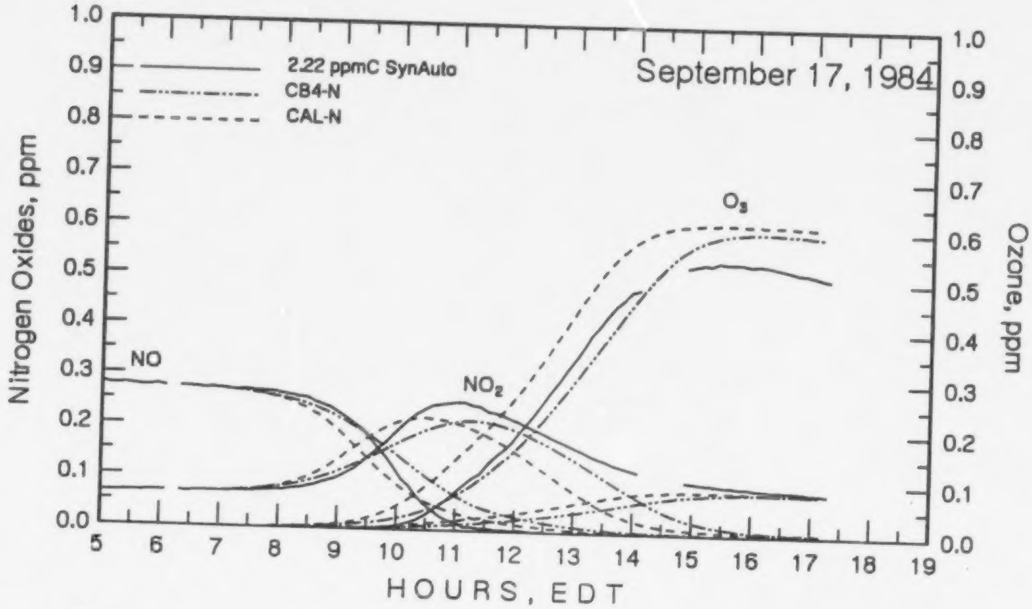


Figure A100. CB4-K and CAL-K Predictions.



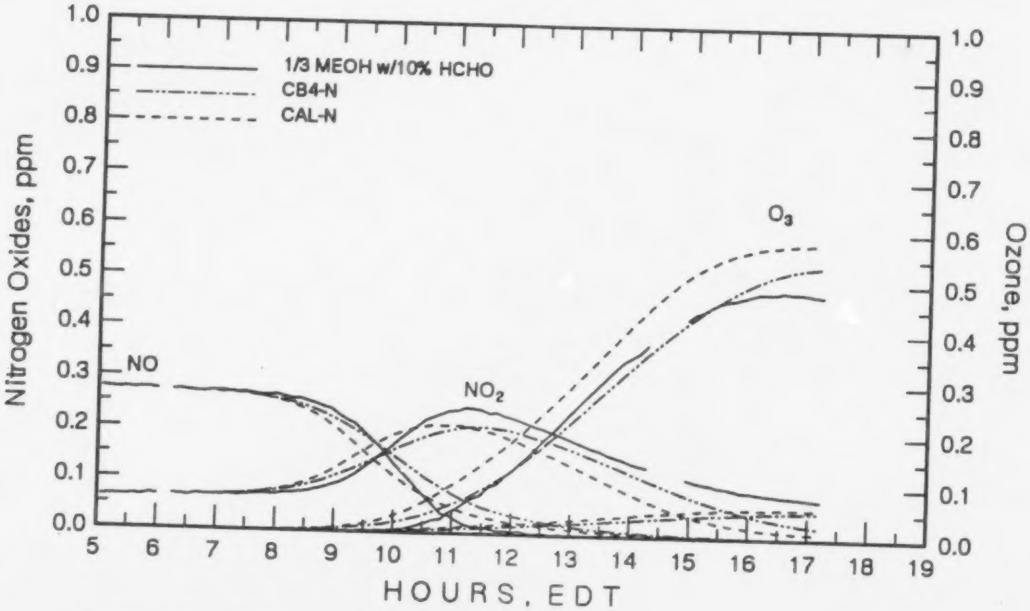


Figure A101. CB4-N and CAL-N Predictions.

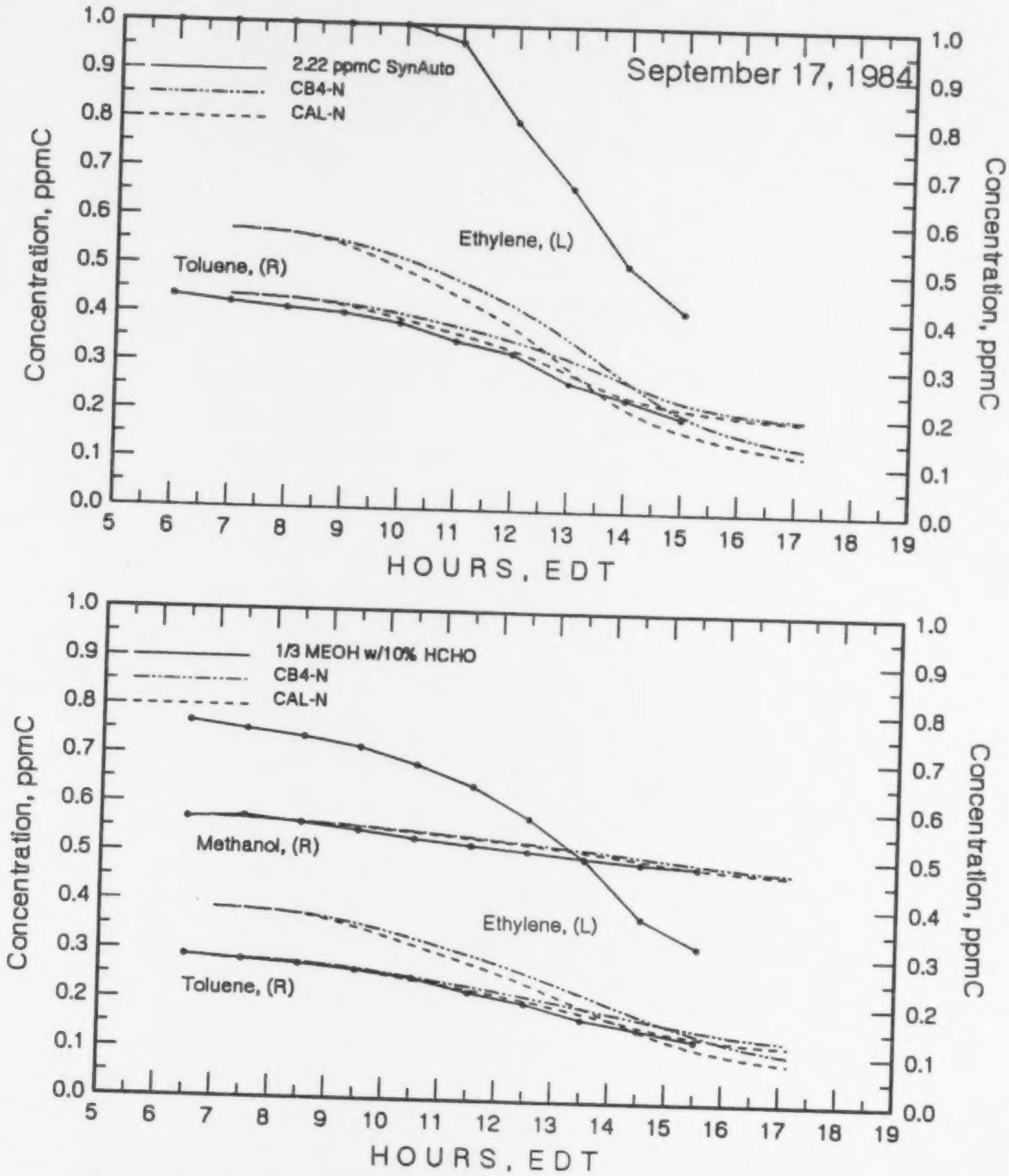


Figure A102. CB4-N and CAL-N Predictions.

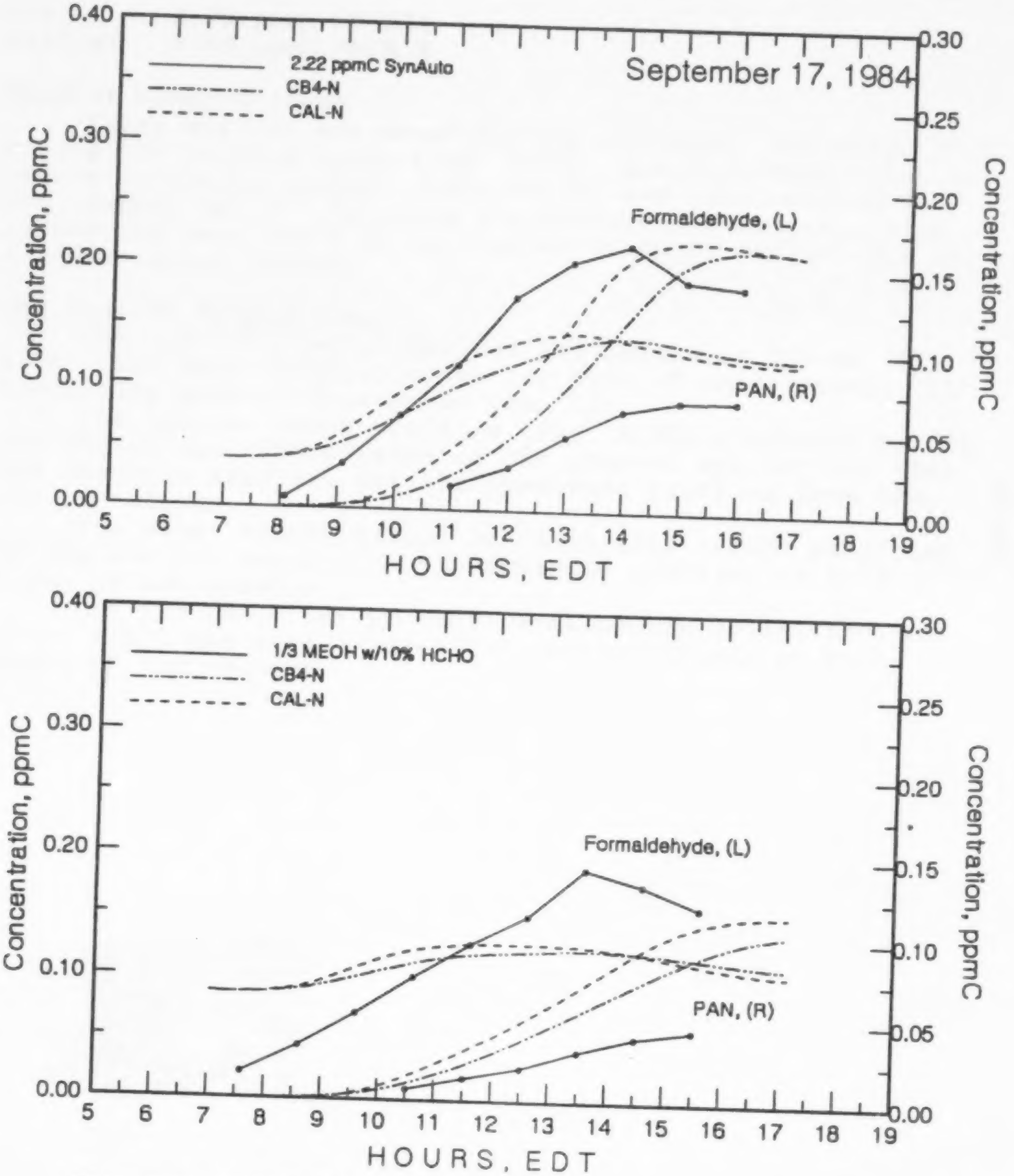


Figure A103. CB4-N and CAL-N Predictions.

September 19, 1984: 40% Hydrocarbon Reduction

Top: 4.38 ppmC HMWMIX
Bottom: 2.69 ppmC HMWMIX

Chamber Observations:

There are not any measurements of chamber humidity during the morning hours (Fig. A104), and therefore, one cannot determine whether condensation may have occured on the chamber walls. Reducing the hydrocarbon concentration caused the peak ozone concentration to occur earlier but at a lower concentration.

CB4 and CAL Predictions:

CB4 and CAL predict earlier NO_x crossover points (Fig. A105) than were observed on either side of the chamber; CAL predicting earlier crossovers than CB4.

The toluene decay profiles (Fig. A106) predicted by CB4 and CAL on the control side of the chamber are earlier than the observed profile, but the predicted profiles have the correct shapes.

The ozone concentration profiles (Fig. A105) predicted by CB4 and CAL agree with the observed profiles on both sides of the chamber.

CB4 and CAL under predict formaldehyde concentrations (Fig. A107) and over predict PAN concentrations on both sides of the chamber.

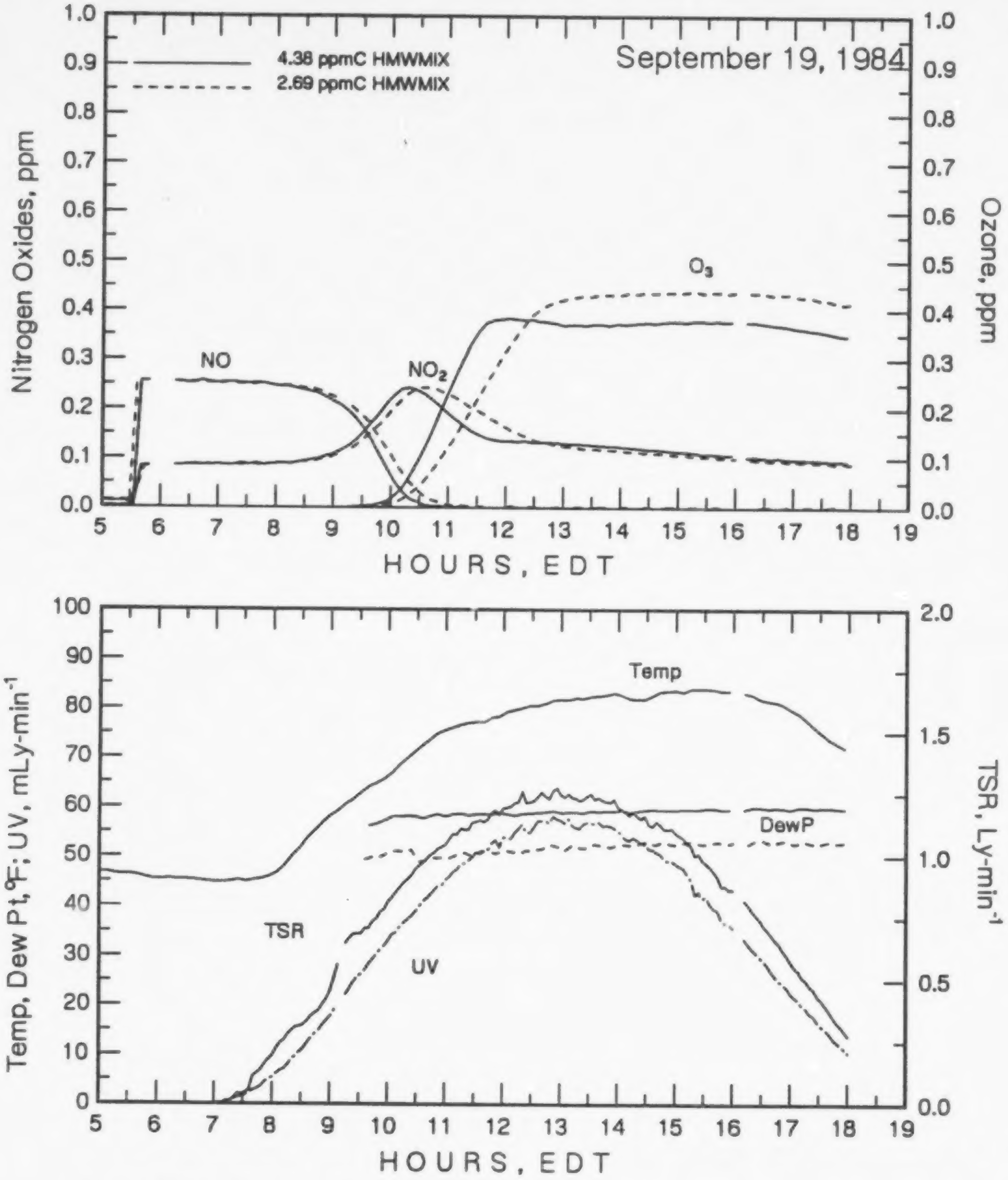
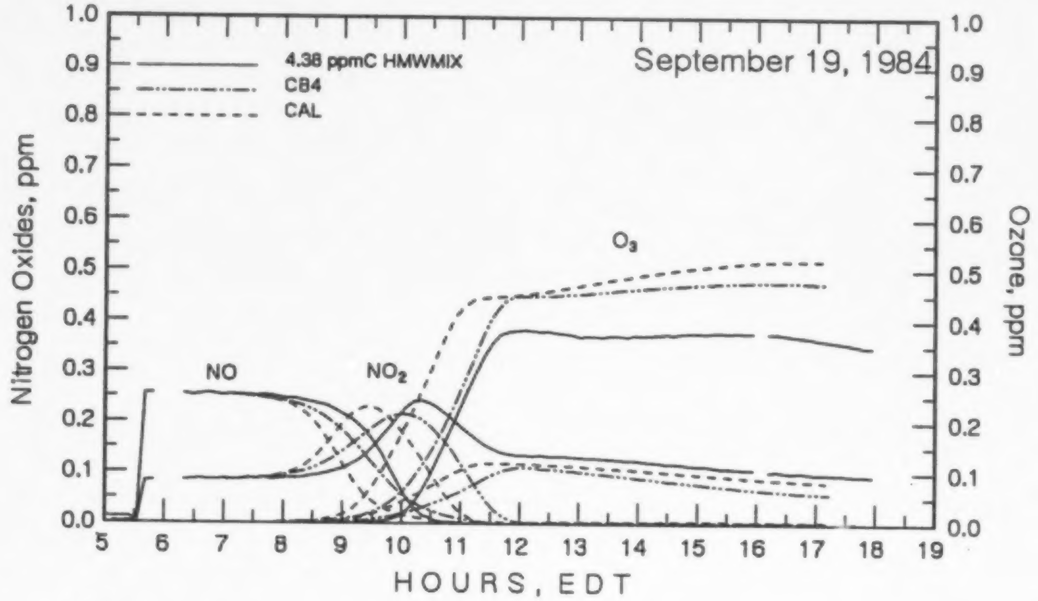


Figure A104. Chamber Observations.



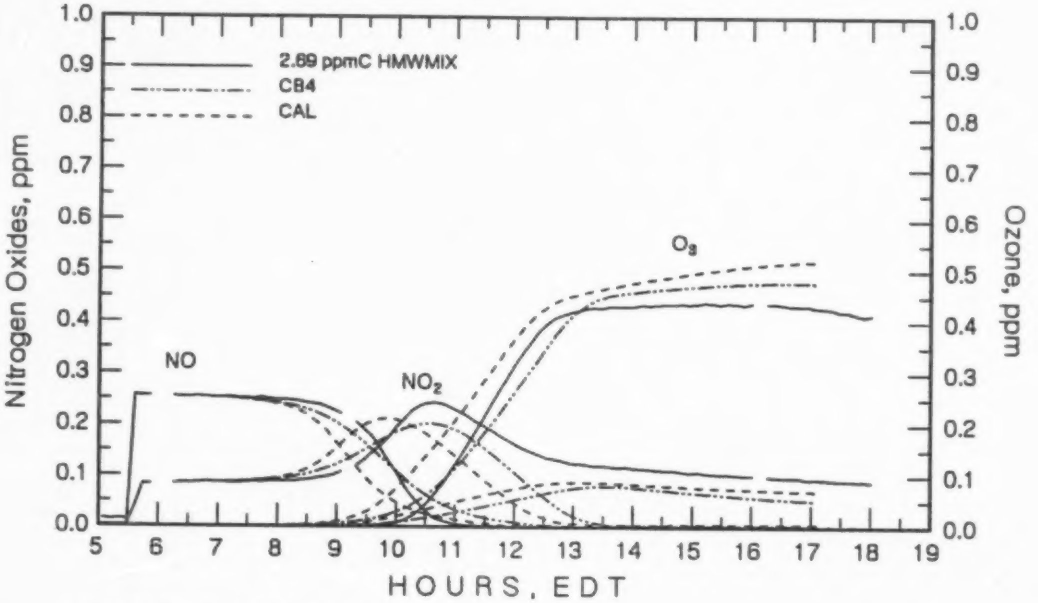


Figure A105. CB4 and CAL Predictions.

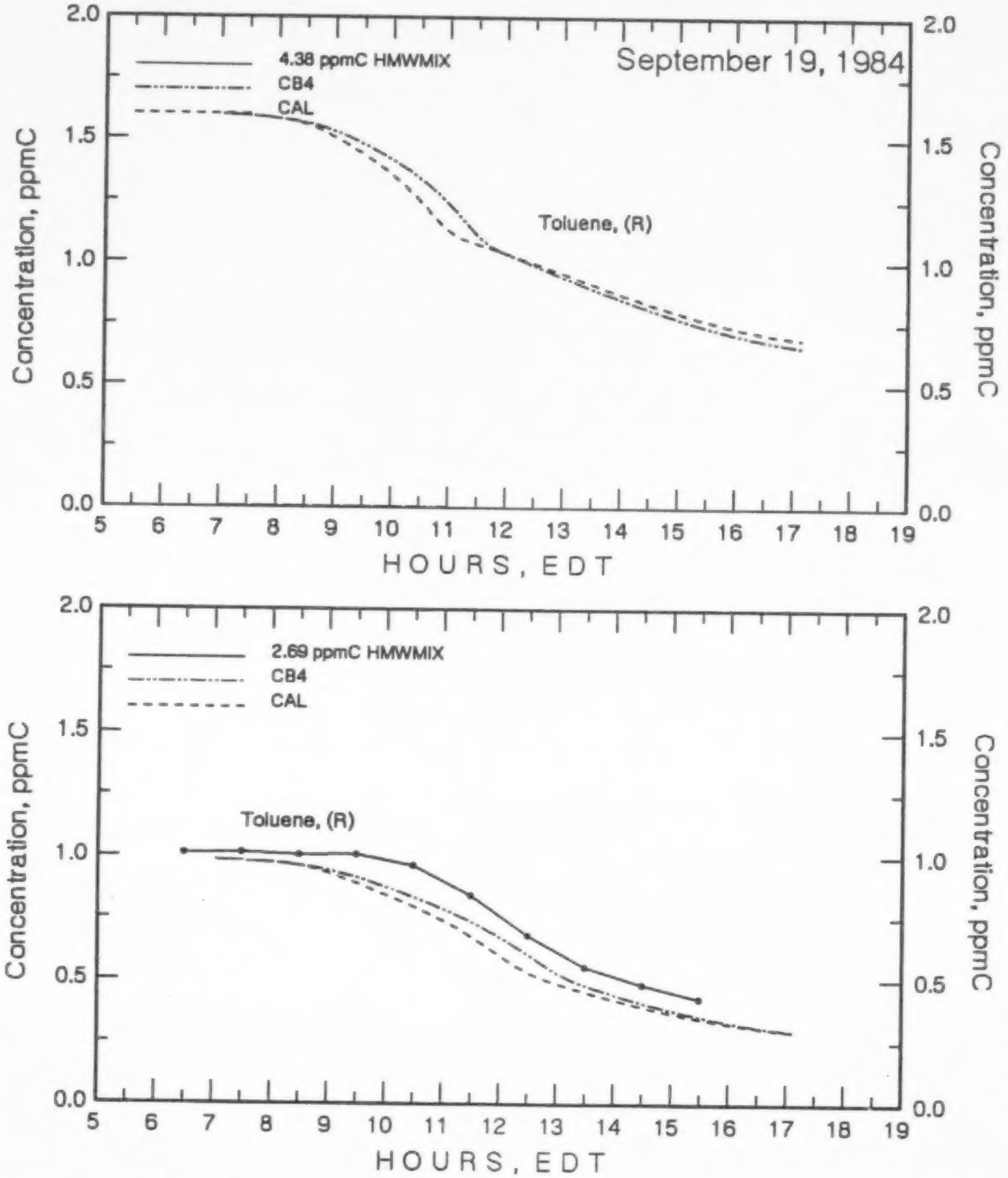


Figure A106. CB4 and CAL Predictions.

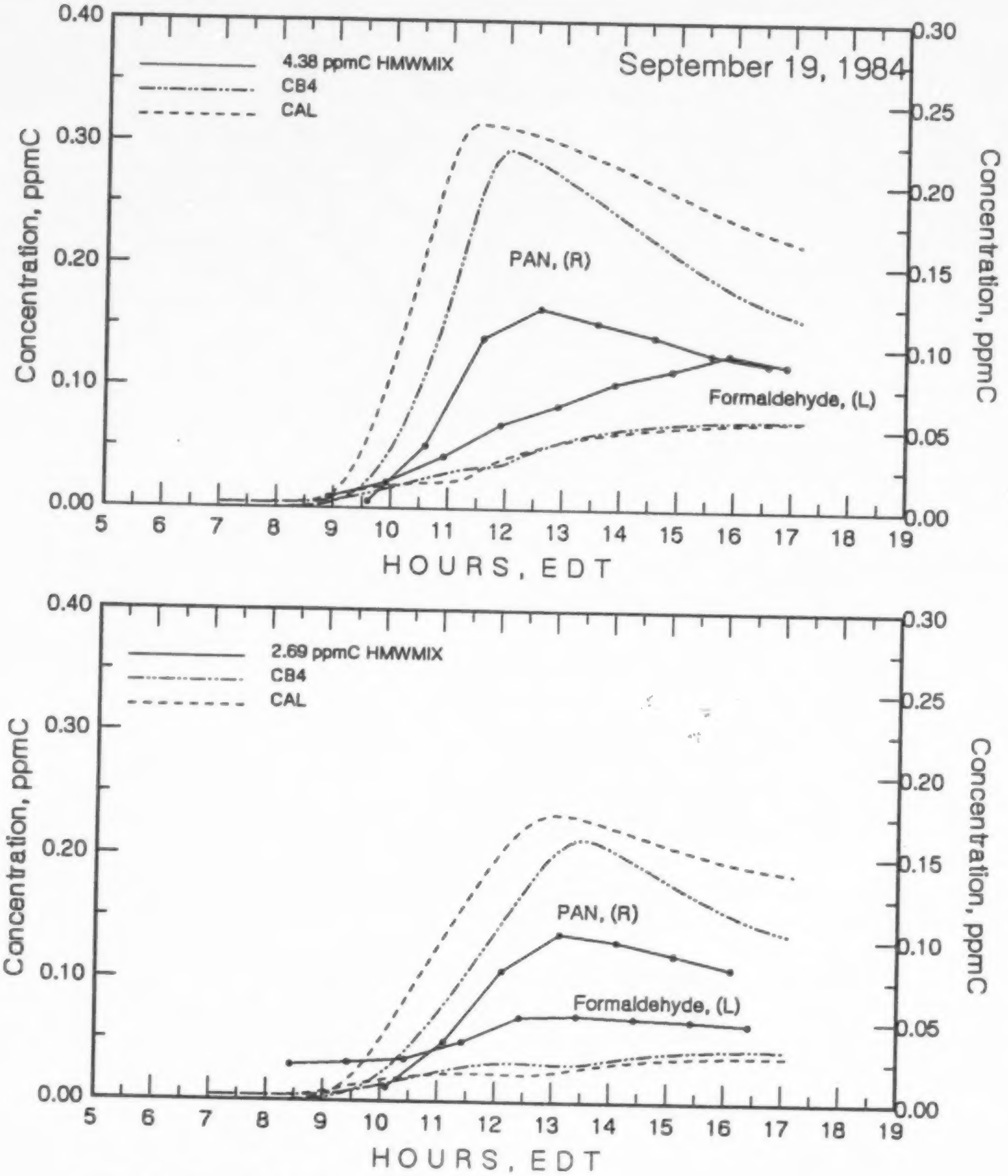


Figure A107. CB4 and CAL Predictions.

September 21, 1984: Formaldehyde Addition

Top: 2.40 ppmC SynAutoUrb
Bottom: 2.40 ppmC SynAutoUrb, 0.18 ppm HCHO

Chamber Observations:

Adding 7.5% formaldehyde caused the NO_x crossover point and ozone production (Fig. A108) to occur earlier with only a slight increase in peak ozone concentration.

CB4 and CAL Predictions:

CB4 and CAL predict earlier NO_x crossover points (Fig. A109) than were observed on either side of the chamber.

The toluene decay profiles (Fig. A110) predicted by CB4 and CAL are correct, but the predicted ethylene decay profiles are steeper than the observed profiles.

As expected from the hydrocarbon decays, CB4 and CAL over predict the peak ozone concentrations (Fig. A109) observed on both sides of the chamber, but the P/O ratios are less than 1.3. The relative change in the peak ozone concentration due to the addition of formaldehyde is slightly underpredicted.

The formaldehyde concentration profiles (Fig. A111) predicted by CB4 and CAL agree with the observed profiles on both sides of the chamber. CB4 and CAL over predict the PAN concentration profiles on both sides of the chamber.

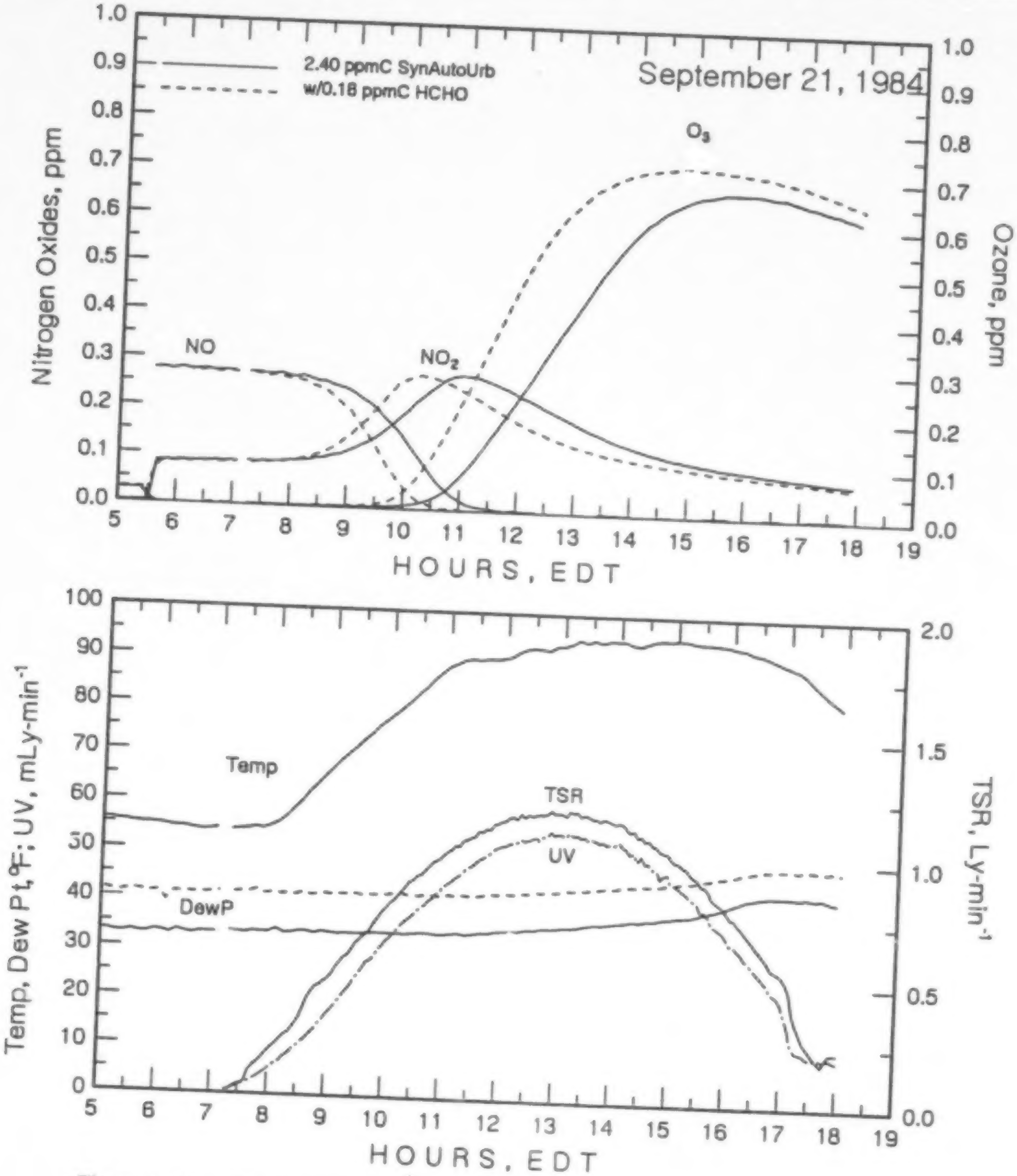


Figure A108. Chamber Observations.

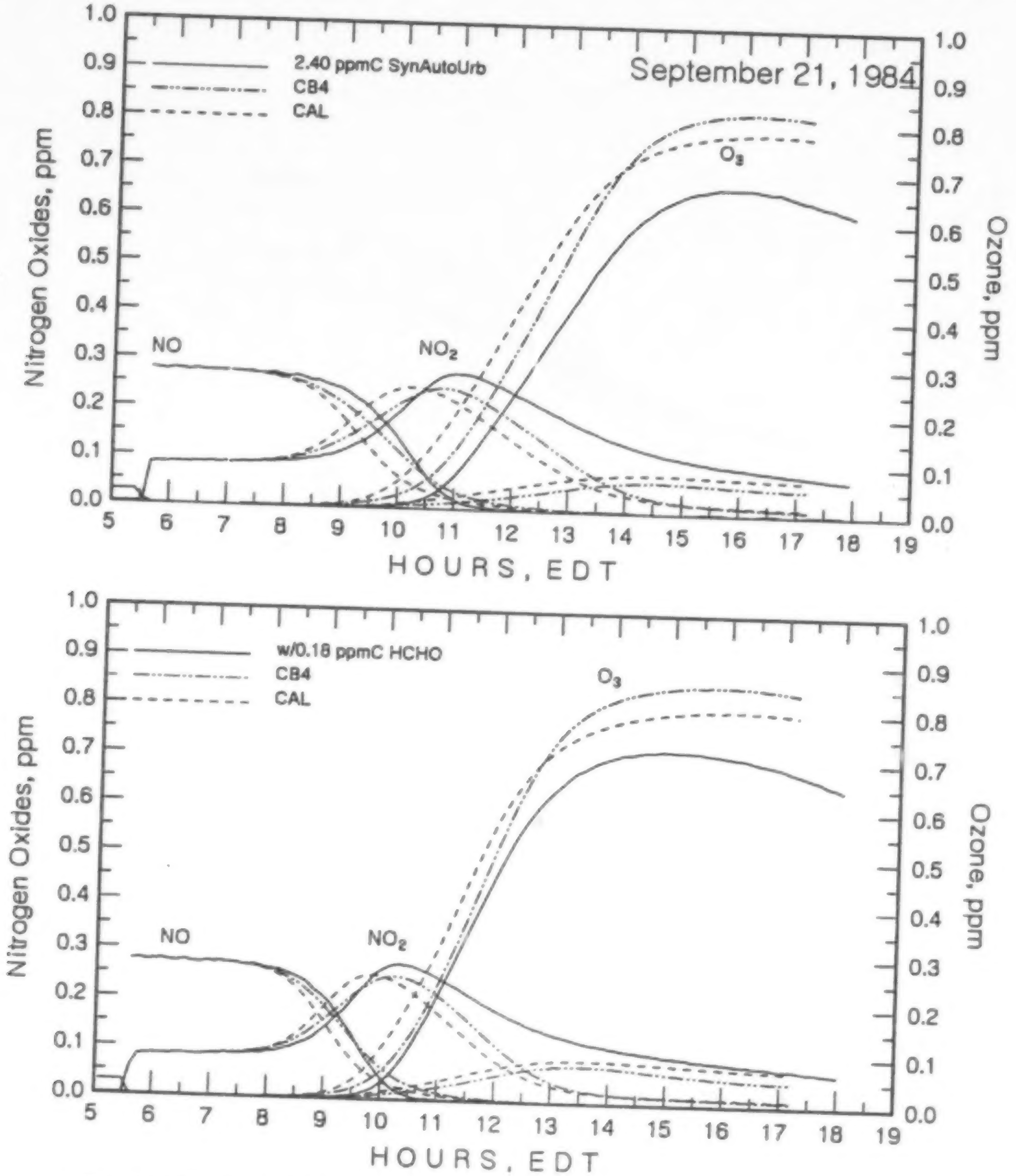


Figure A109. CB4 and CAL Predictions.

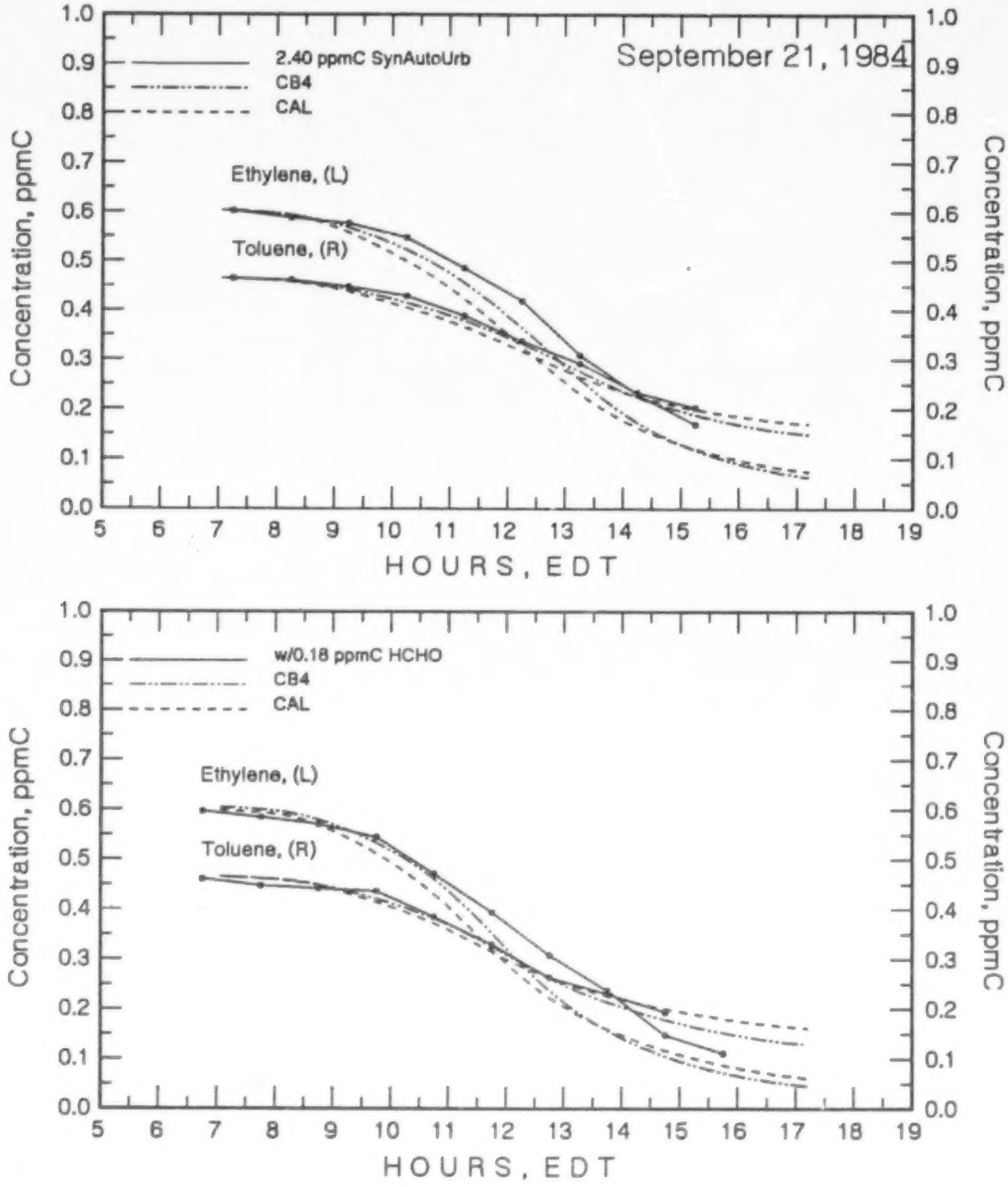


Figure A110. CB4 and CAL Predictions.

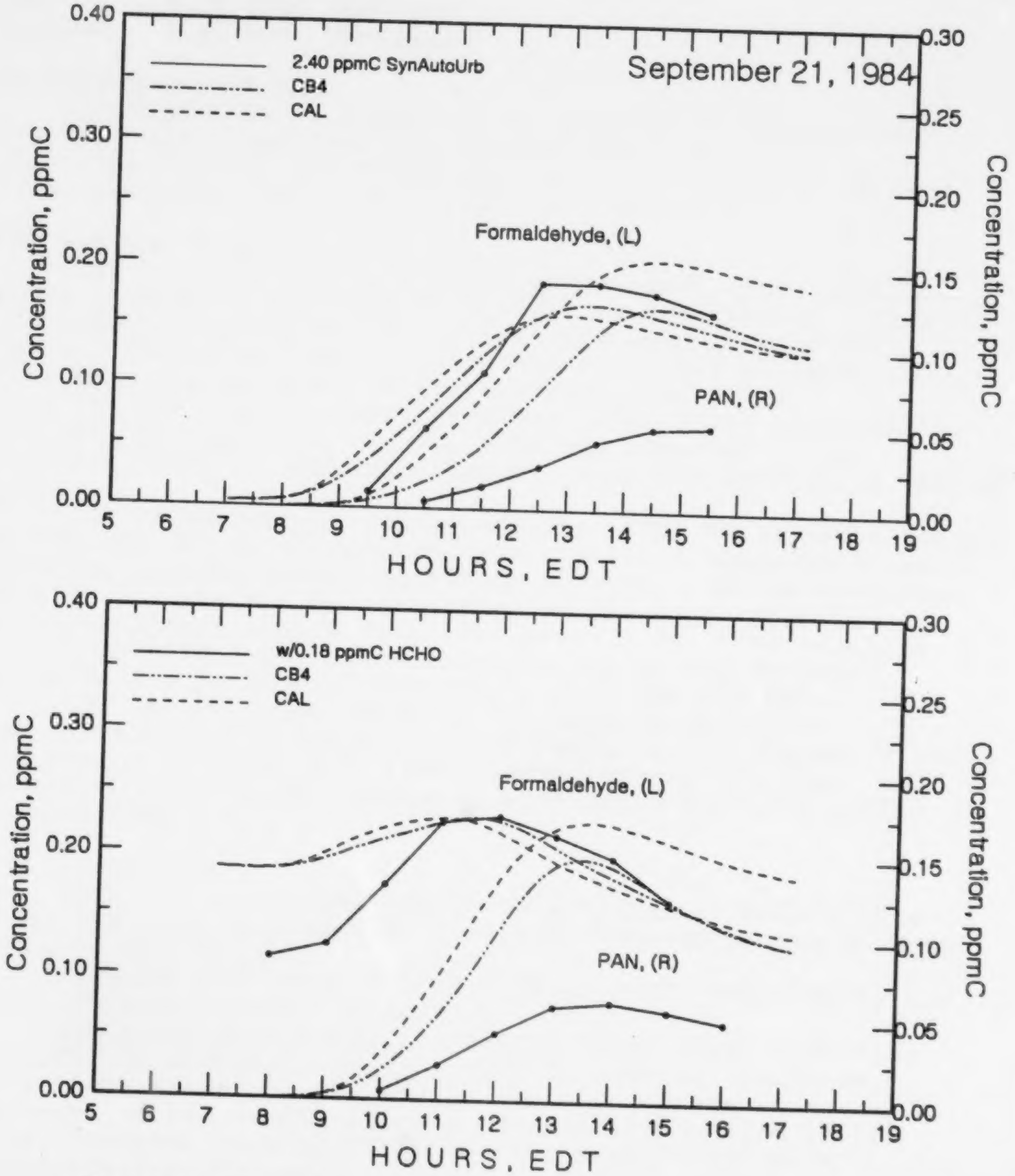


Figure A111. CB4 and CAL Predictions.

June 26, 1985: 1/3 Hydrocarbon Reduction

Top: 2.27 ppmC SynUrban
Bottom: 3.10 ppmC SynUrban

Chamber Observations:

In Figure A112, there are no temperature observations for this day. Reducing the initial hydrocarbon concentrations by one third resulted in a reduction in peak ozone concentration from 0.8 ppm to 0.64 ppm.

CB4 and CAL Predictions:

CAL predicts NO_x crossover points (Fig. A113) that are about 40 minutes early on both sides of the chamber, while CB4 predicts crossover points that are only 20 minutes early. Therefore, one expects that the model predictions will be early compared to the observed conditions.

The hydrocarbon decay profiles (Fig. A114) predicted by CB4 and CAL replicate the shape of the observed decay profiles well; as expected, though, they are shifted to the left.

The ozone concentration profiles (Fig. A113) predicted by CB4 and CAL on the control side (bottom) agree with the observed profile given the timing problem. On the reduction side (top), CB4 and CAL over predict the ozone peak concentration with P/O ratios of about 1.25. The relative change in peak ozone concentrations due to the methanol substitution is under estimated by both CB4 and CAL.

CB4 and CAL under predict the peak formaldehyde concentration (Fig. A115) on both sides of the chamber with P/O ratios of about 0.5. PAN concentrations are over predicted by both mechanisms on both sides with P/O ratios greater than 2.

CIT Predictions:

Both CIT mechanisms predict NO_x crossover points (Fig. A116) one half hour earlier that the observed points on both sides of the chamber.

The ethylene decay profiles (Fig. A117) produced by the CIT mechanisms appear correct.

The ozone concentration profile (Fig. A116) predicted by CIT-1 is obviously wrong. CIT-2, however, performs quite well except at the end of the day. There is no decrease in the predicted rate of ozone production in the late afternoon causing CIT-2 to over predict the peak concentration of ozone.

Although the peak formaldehyde concentrations (Fig. A118) predicted by CIT-1 may agree well with the observed peaks, the shape of the predicted profiles are wrong. CIT-2 under predicts the formaldehyde concentration profiles with P/O ratios of aprroxiamately 0.5 on both sides of the chamber. CIT-1 under predicts PAN concentrations with P/O ratios of 0.4 and 0.3 on the reduction (top) and control (bottom) sides, respectively. CIT-2 produces P/O ratios of 0.2 and 0.15, respectively.

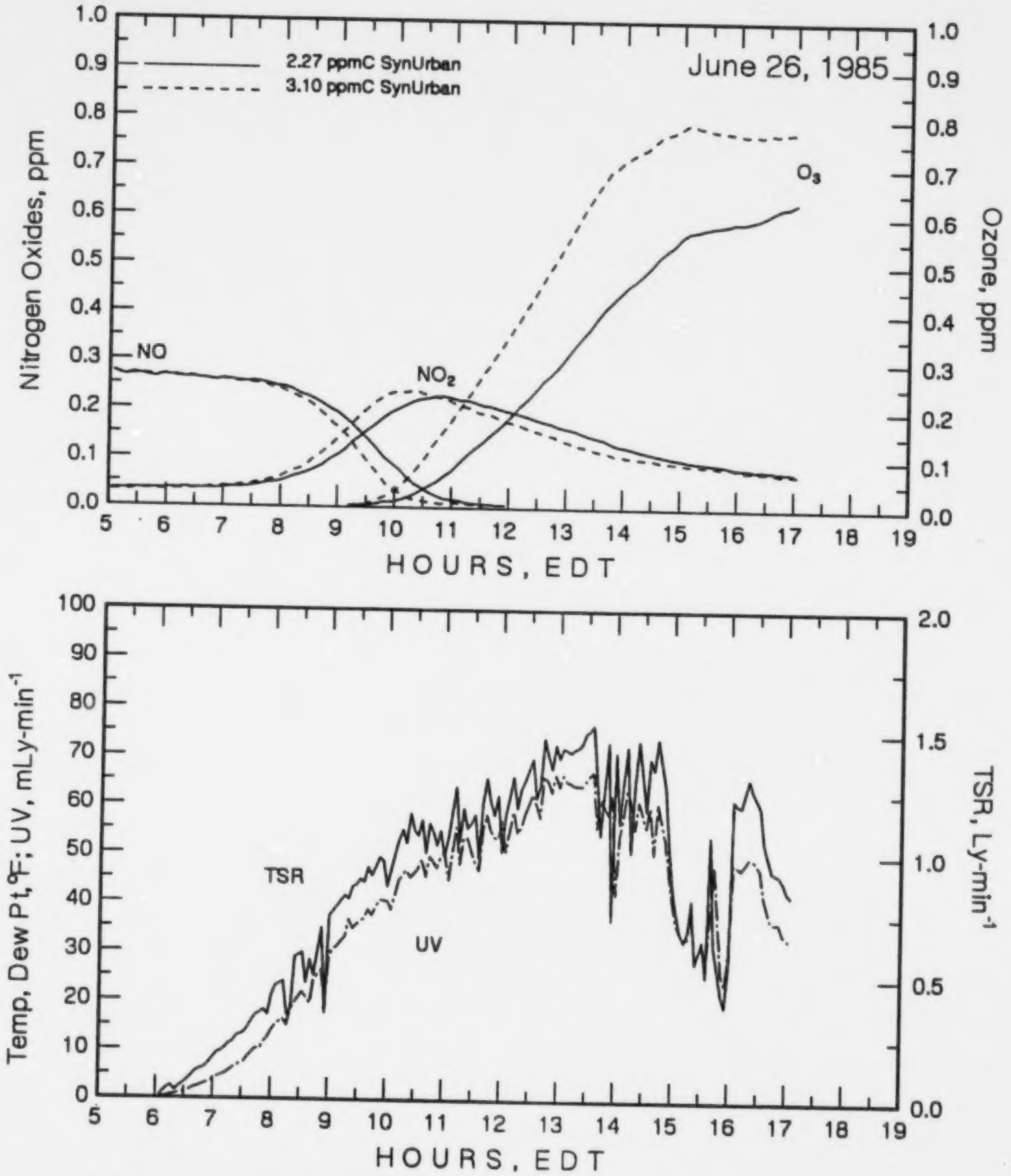


Figure A112. Chamber Observations.

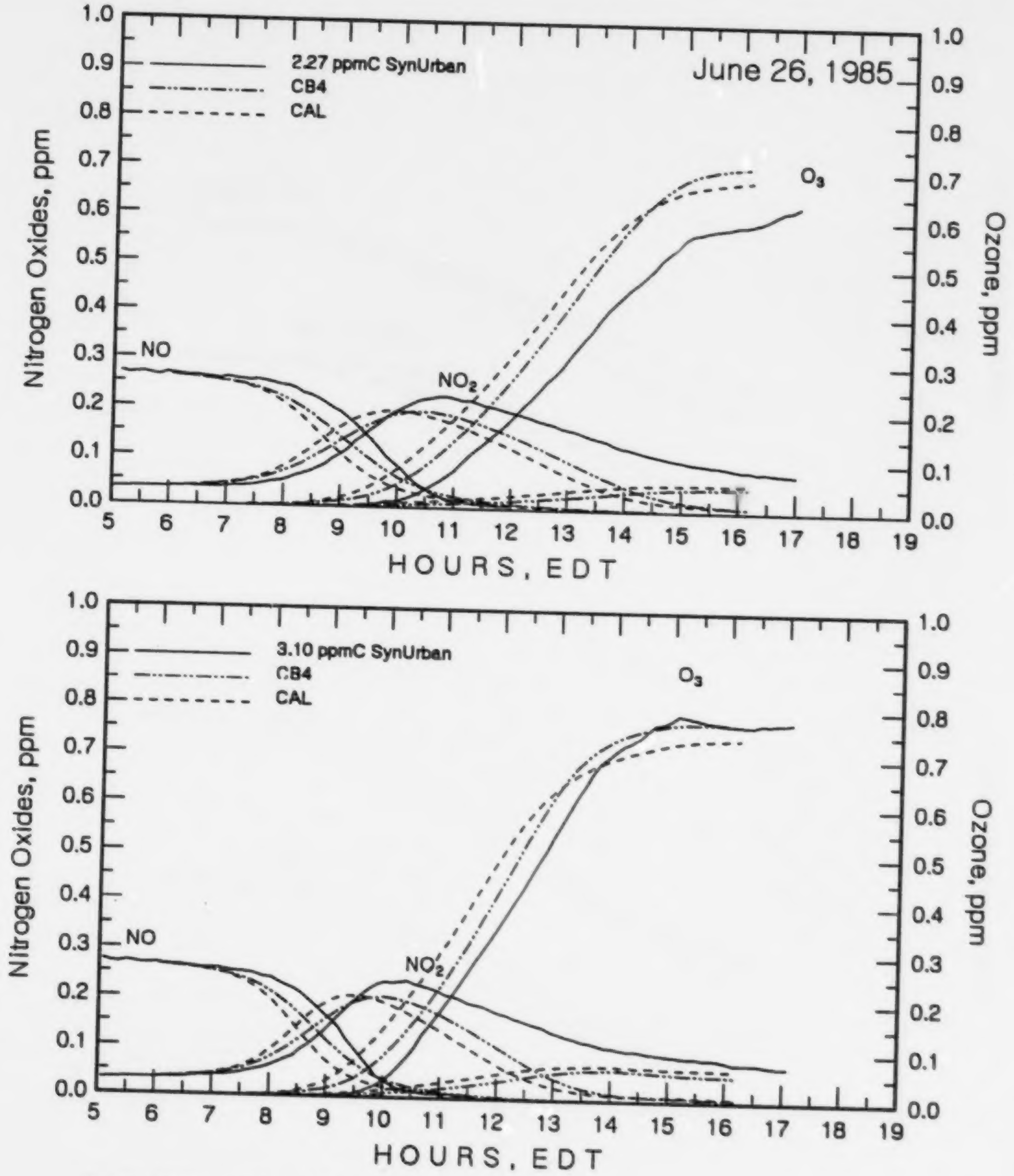


Figure A113. CB4 and CAL Predictions.

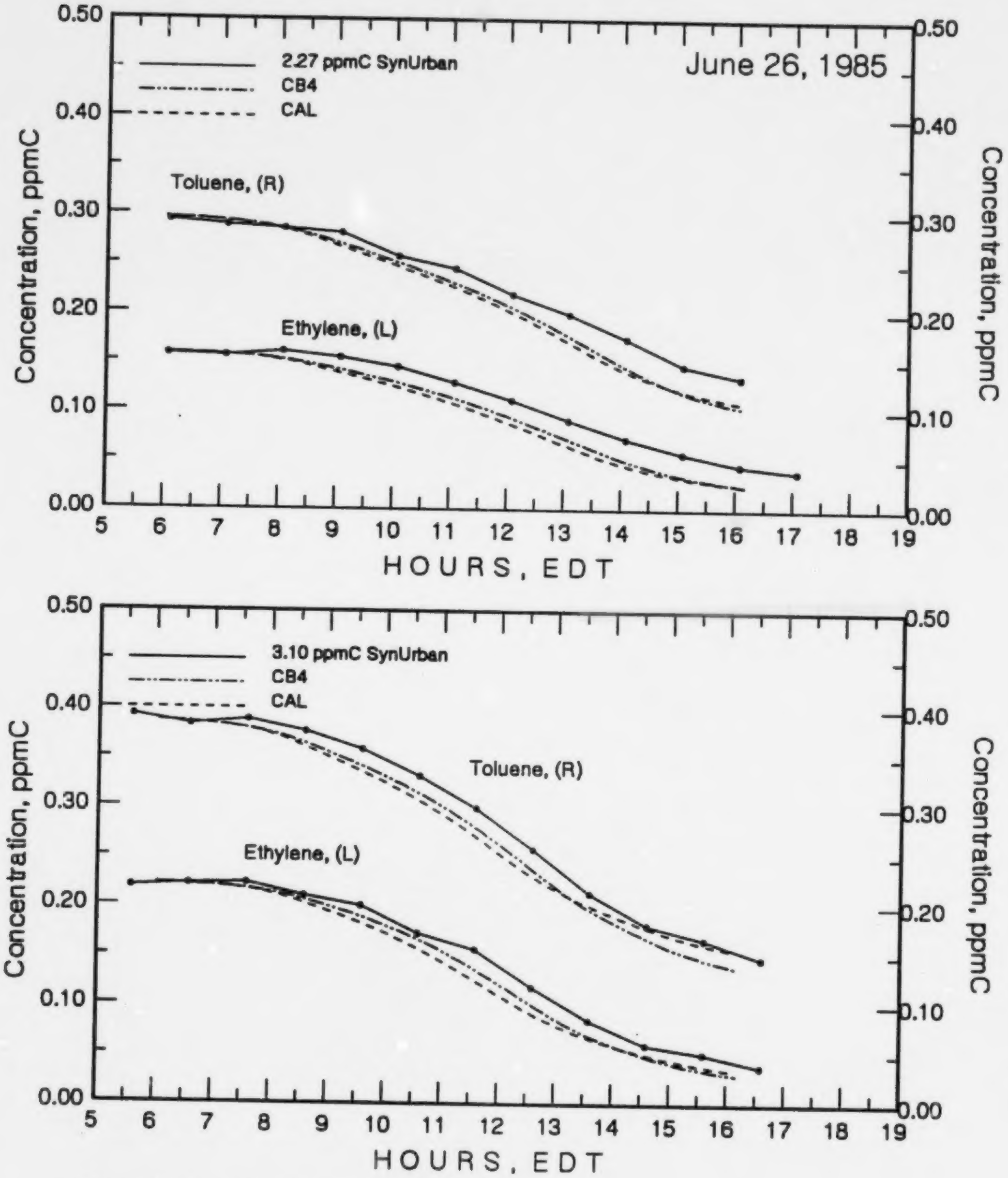


Figure A114. CB4 and CAL Predictions.

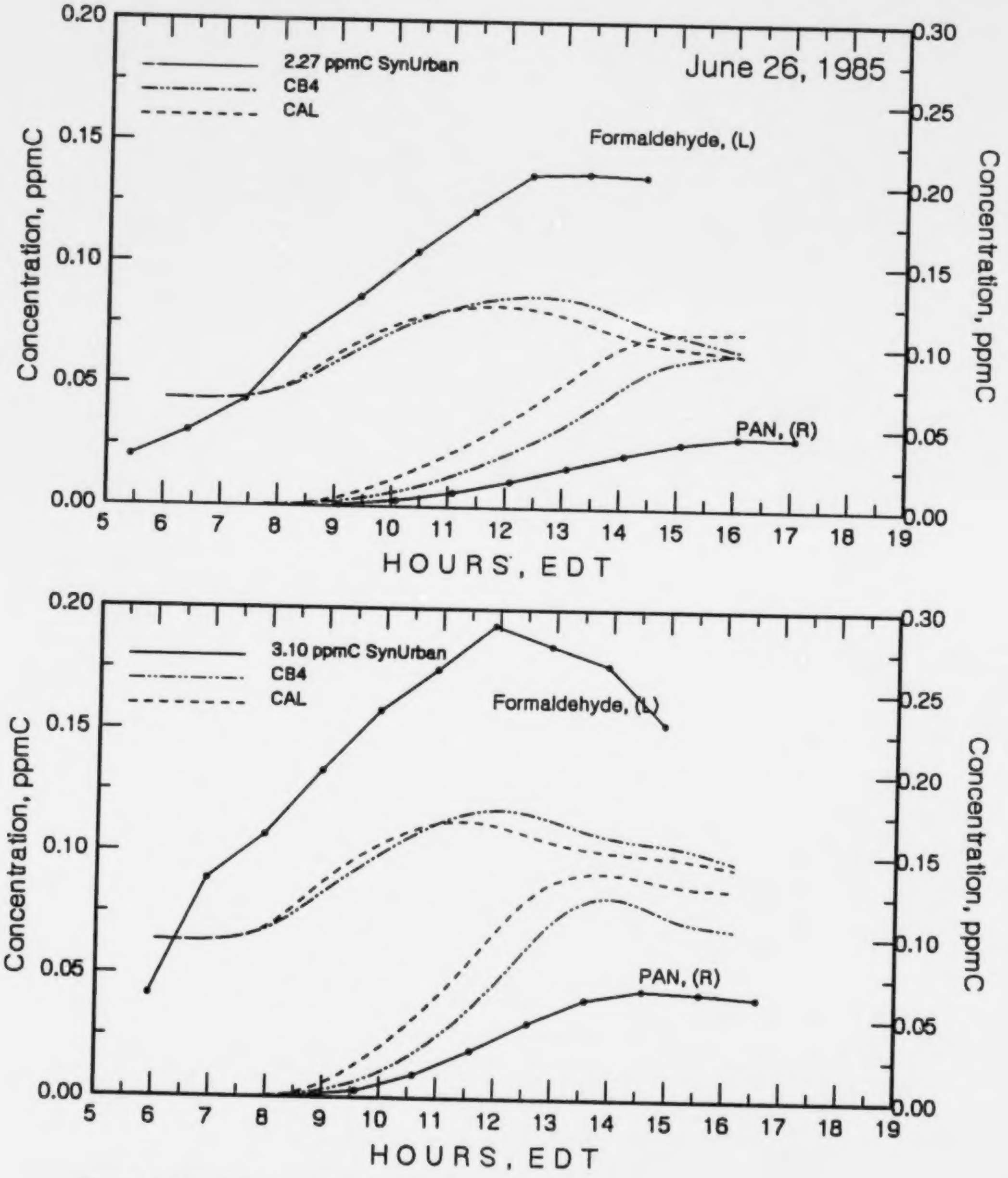
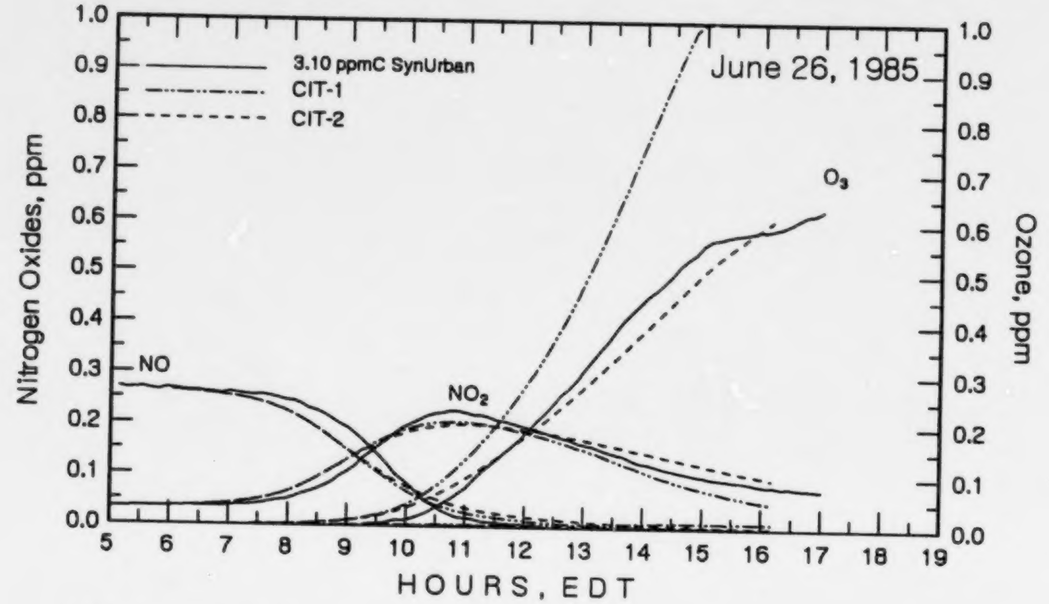


Figure A115. CB4 and CAL Predictions.



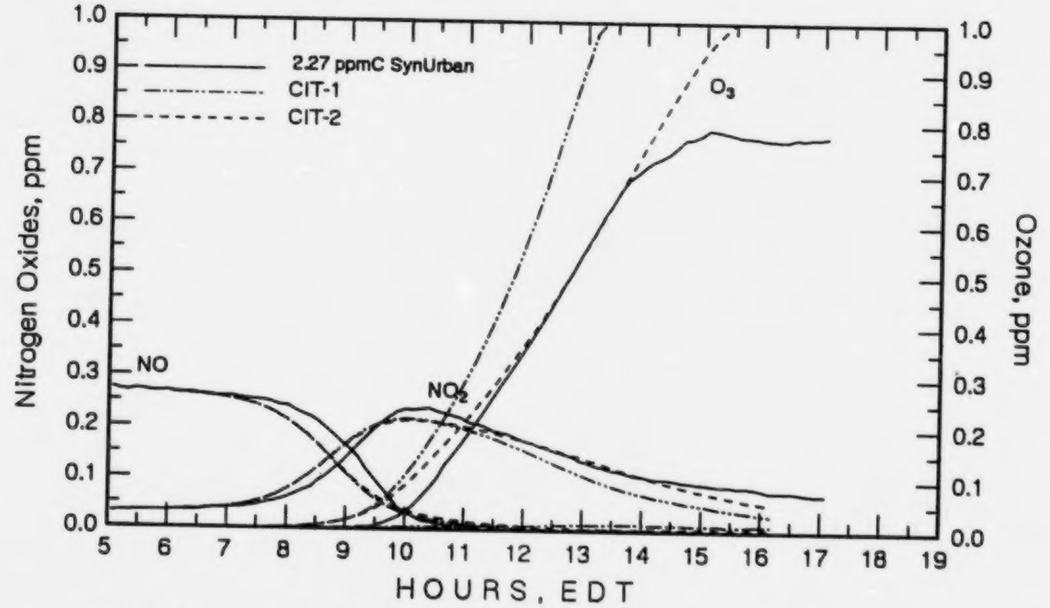
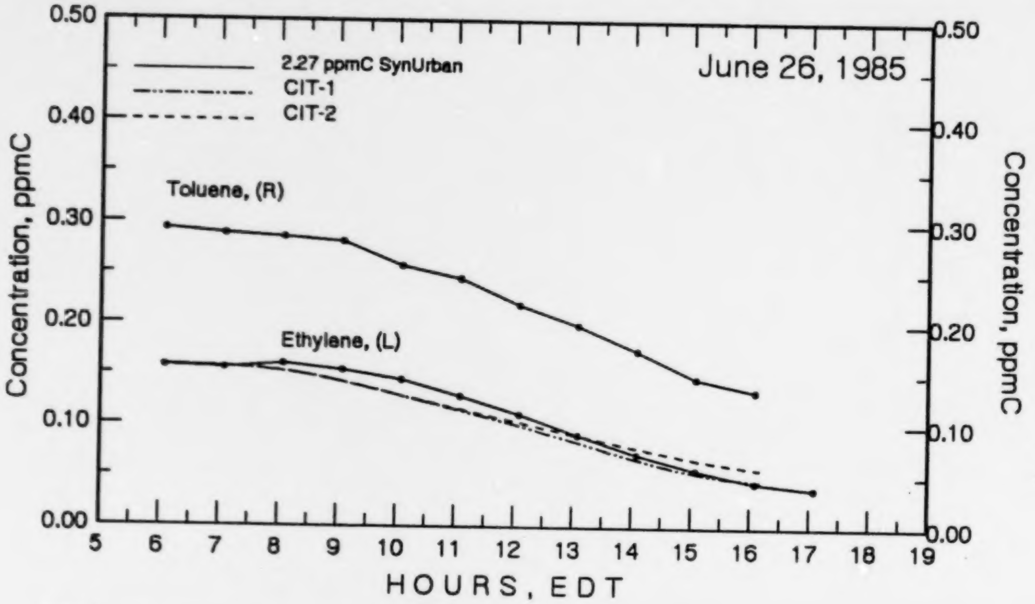


Figure A116. CIT Predictions.



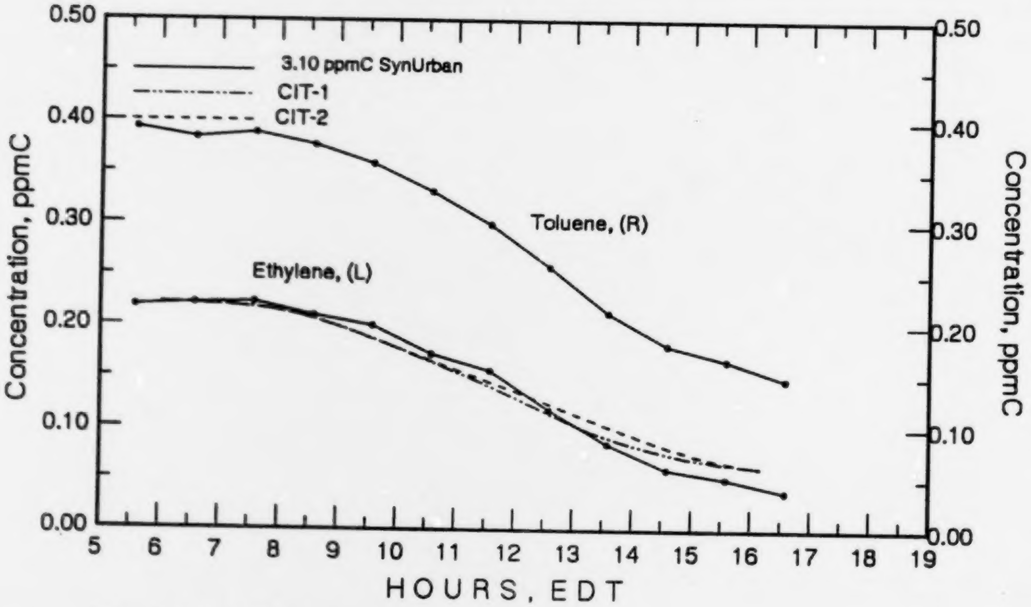


Figure A117. CIT Predictions.

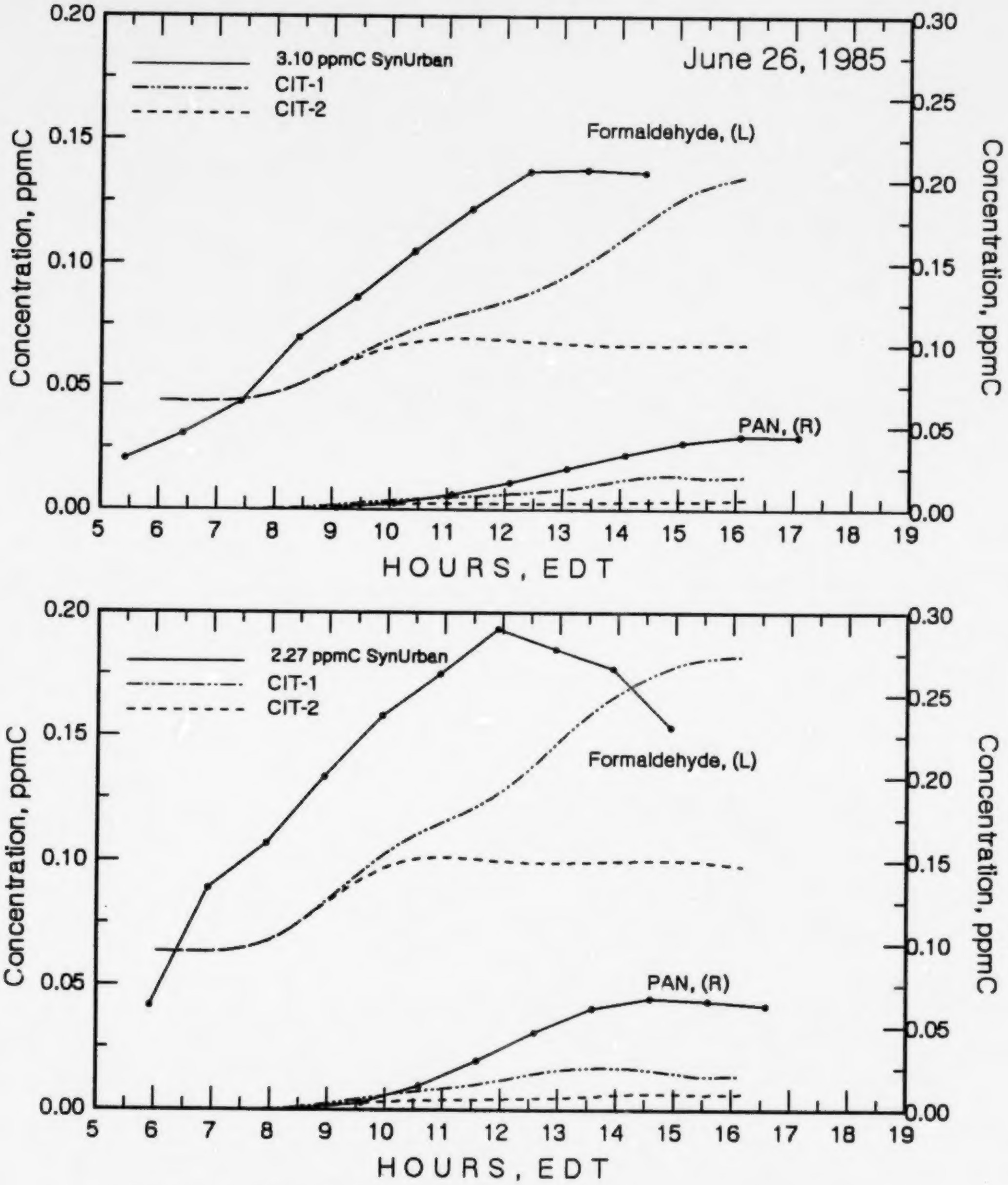


Figure A118. CIT Predictions.

June 28, 1985: 1/3 Methanol Substitution w/10% HCHO

Top: 2.4 ppmC SynUrban
Bottom: 1.3 ppmC SynUrban, 0.6 ppm MEOH, 0.07 ppm HCHO

Chamber Observations:

In Figure A119, there are no temperature observations plotted for this day. The effect of the methanol substitution was actually to increase the peak ozone concentration from 0.24 ppm to 0.28 ppm.

CB4 and CAL Predictions:

The NO_x crossover points (Fig. A120) predicted by CB4 and CAL are early compared to the observed crossover points.

Given the timing problem, the predicted hydrocarbon decay profiles (Fig. A121) appear to be adequate for the control side (top). On the substitution side (bottom), CB4 and CAL predict faster hydrocarbon decays than was observed. Therefore, one expects the models to predict higher ozone concentrations than were observed on the substitution side.

CB4 and CAL over predict the ozone concentrations (Fig. A120) on the control side (top) with P/O ratios of 1.7 and 2, respectively. On the substitution side (bottom), where poorer performance was expected, CB4 and CAL produce P/O ratios of 1.1 and 1.25, respectively. Both models predict a relative decrease in ozone concentrations due to the methanol substitution when a increase in the peak ozone concentration was actually observed.

There is a lot of noise in the observed formaldehyde concentration profile (Fig. A122). CB4 and CAL, however, adequately represent the general trend that appears on the control side (top), but they under predict the general trend on the substitution side (bottom). Both CB4 and CAL over predict the PAN concentrations on both sides with P/O ratios greater than 2.

CIT Predictions:

The CIT mechanisms predict that NO_x crossover points (Fig. A123) occur one hour earlier that the observed crossover points.

The ethylene decay profiles (Fig. A124) predicted by the CIT mechanisms are very close to those predicted by CB4 and CAL.

The ozone concentration profiles (Fig. A123) predicted by CIT-1 is much too high. CIT-2 performs better than CB4 and CAL on the control side (top) with a P/O ratio of 1.3. On the substitution side (bottom), CIT-2 performs worse than CB4 and CAL over predicting the peak ozone concentration with a P/O ratio of 1.4.

CIT-1 tracks the noisy formaldehyde concentration profile (Fig. A125) well on both sides of the chamber. CIT-2 under predicts the formaldehyde concentration profile on both sides. CIT-1 also performs well when compared to the PAN concentrations profiles on both sides. CIT-2 greatly under predicts the peak PAN concentrations with P/O ratios equal to 0.1 on both sides of the chamber.

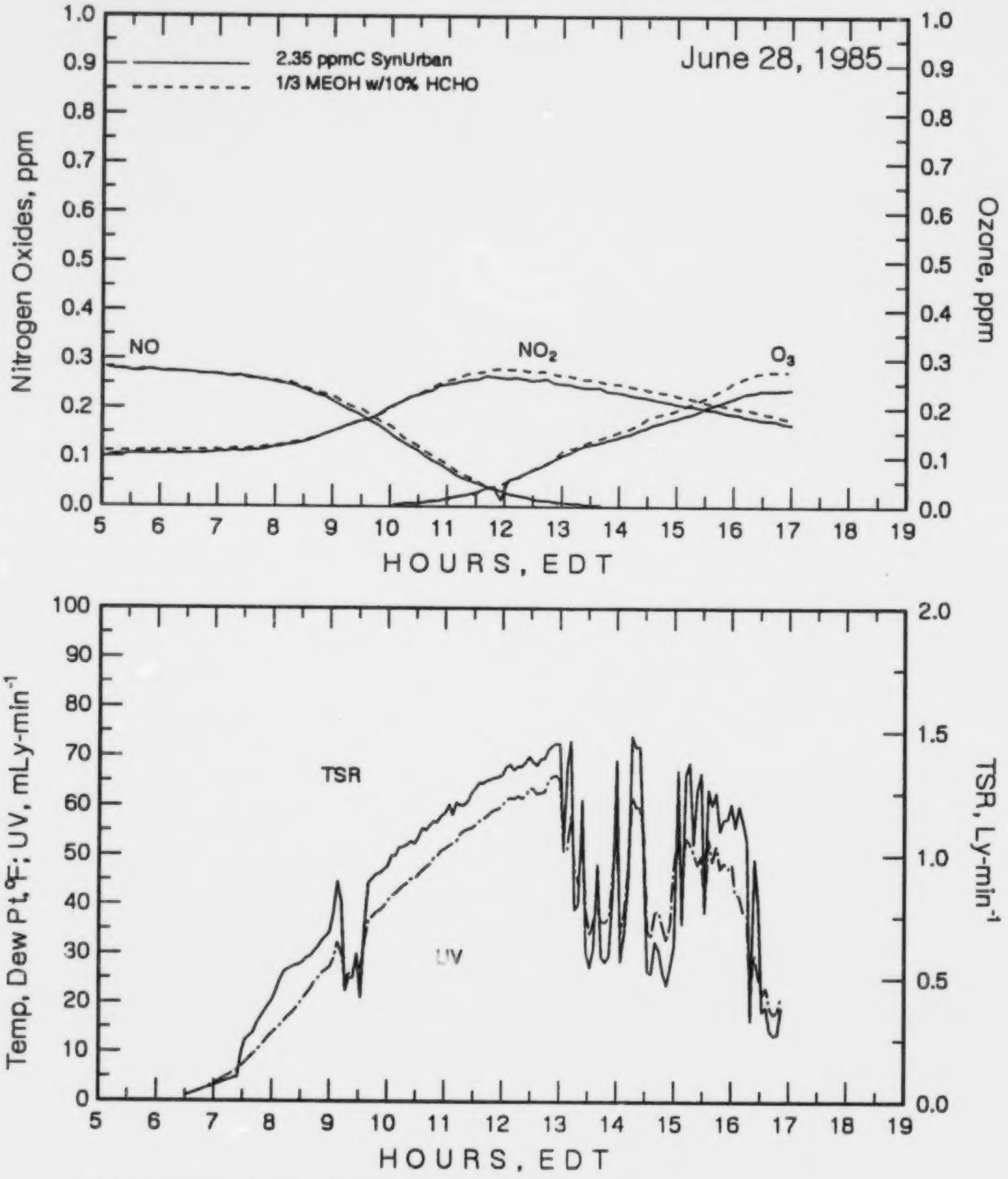


Figure A119. Chamber Observations.

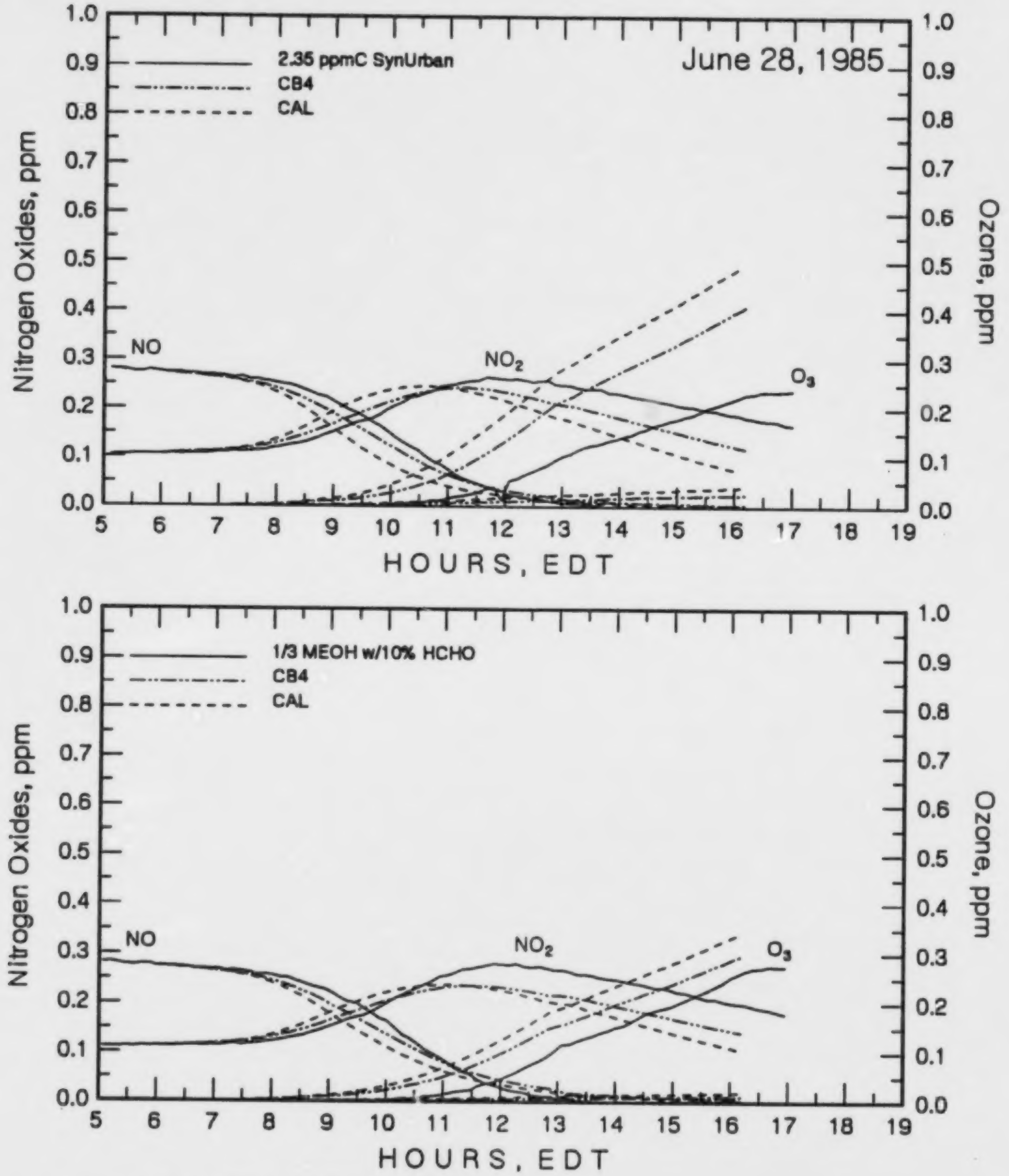


Figure A120. CB4 and CAL Predictions.

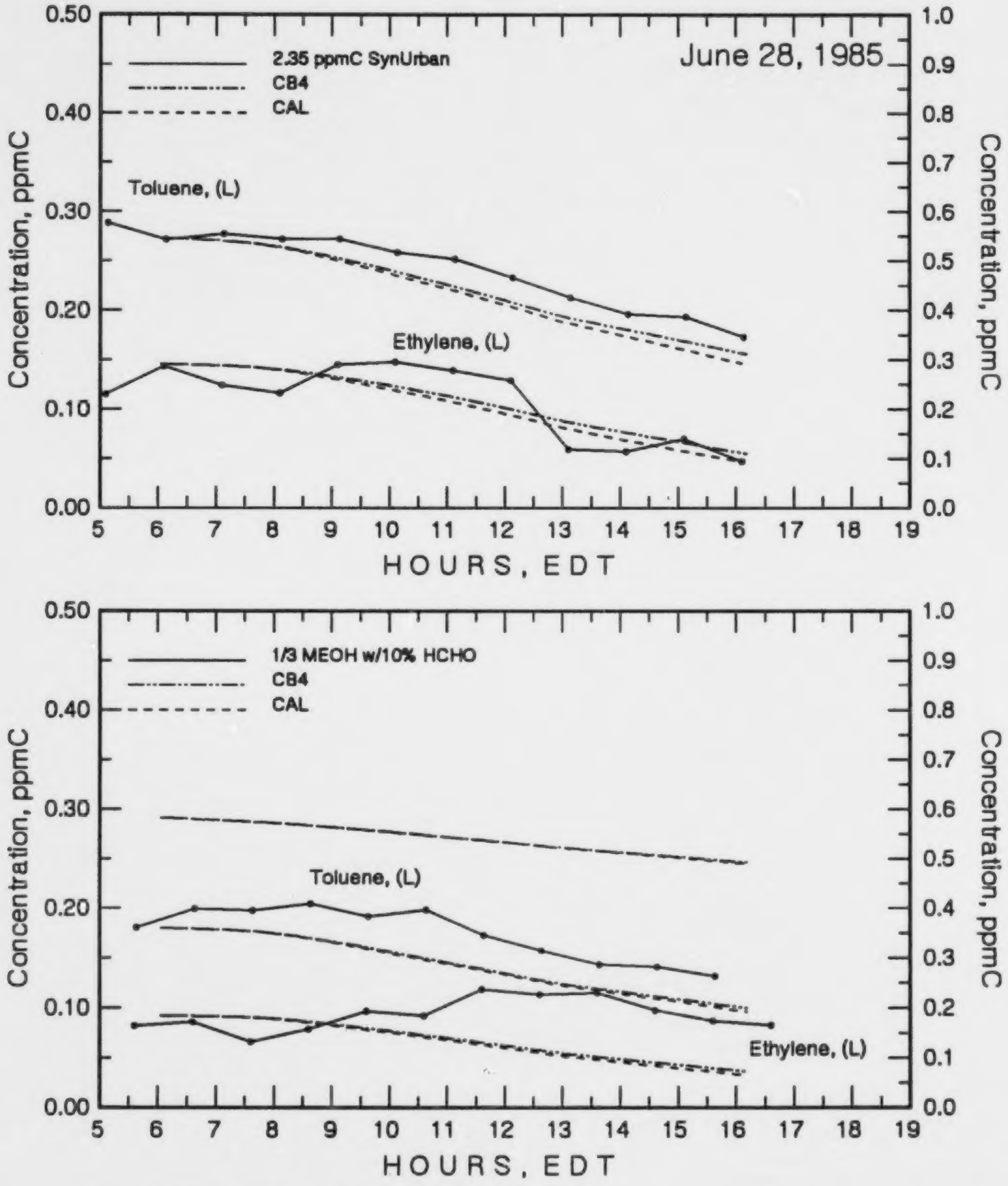


Figure A121. CB4 and CAL Predictions.

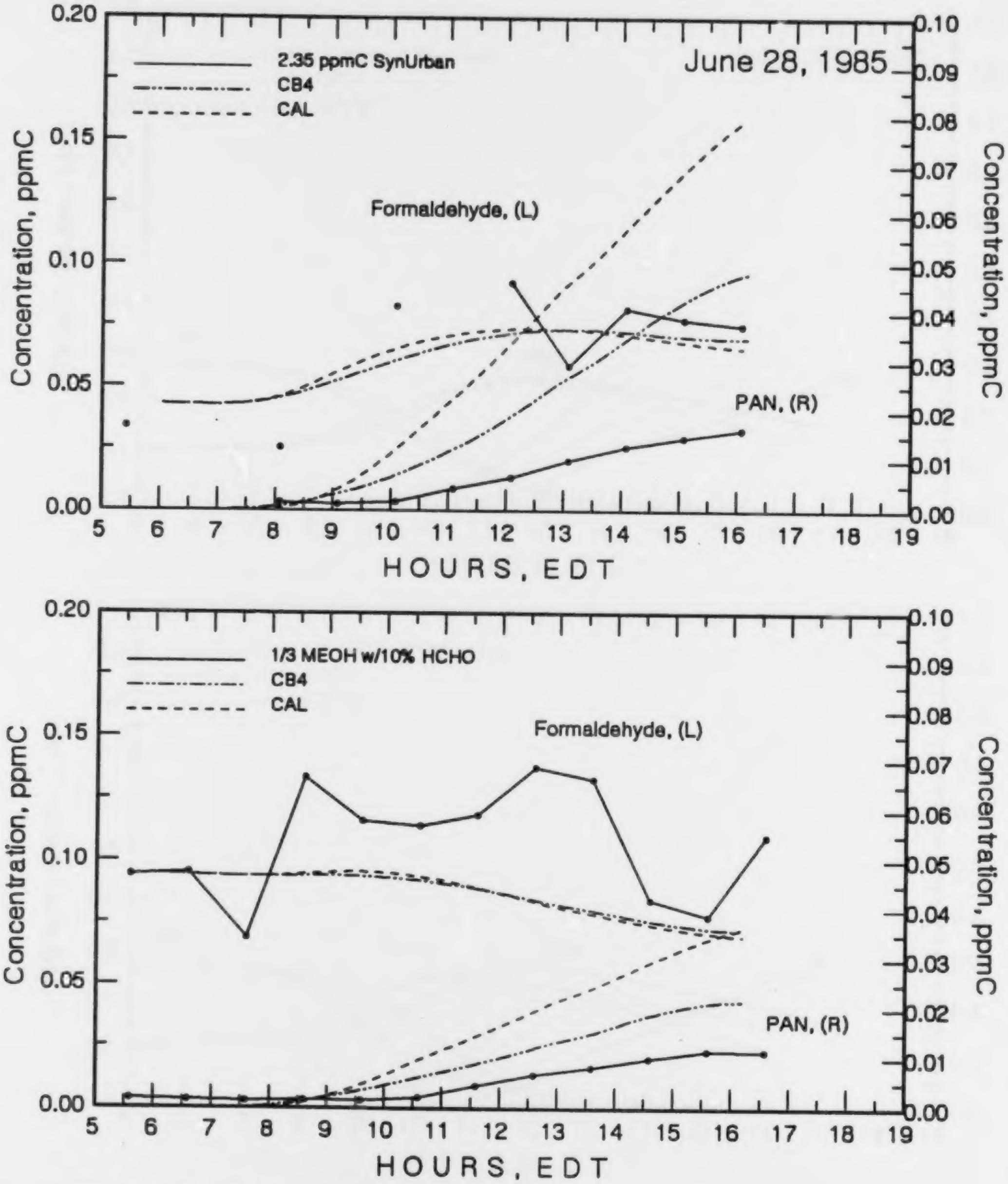
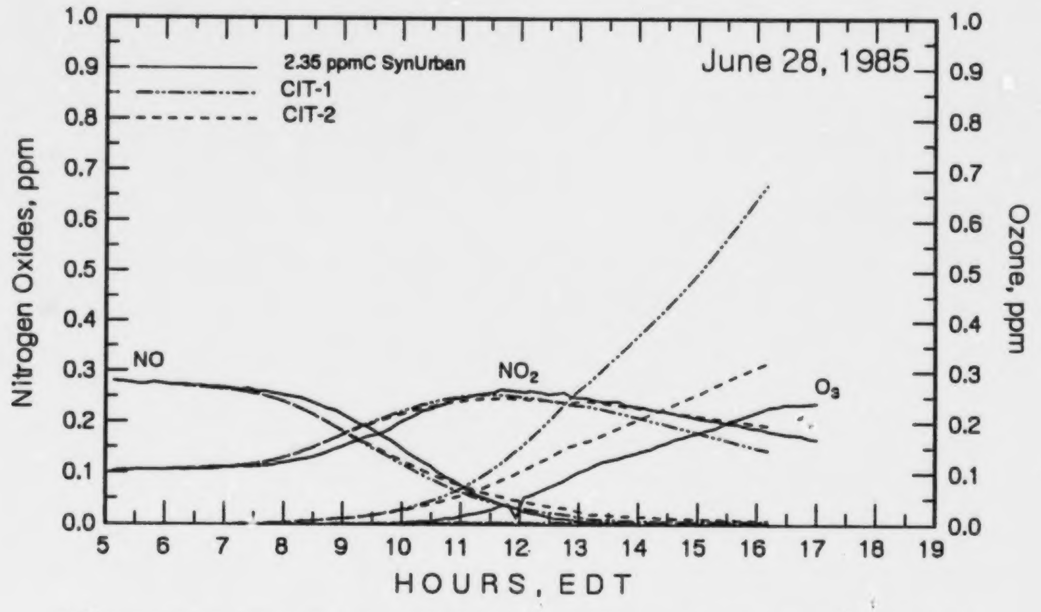


Figure A122. CB4 and CAL Predictions.



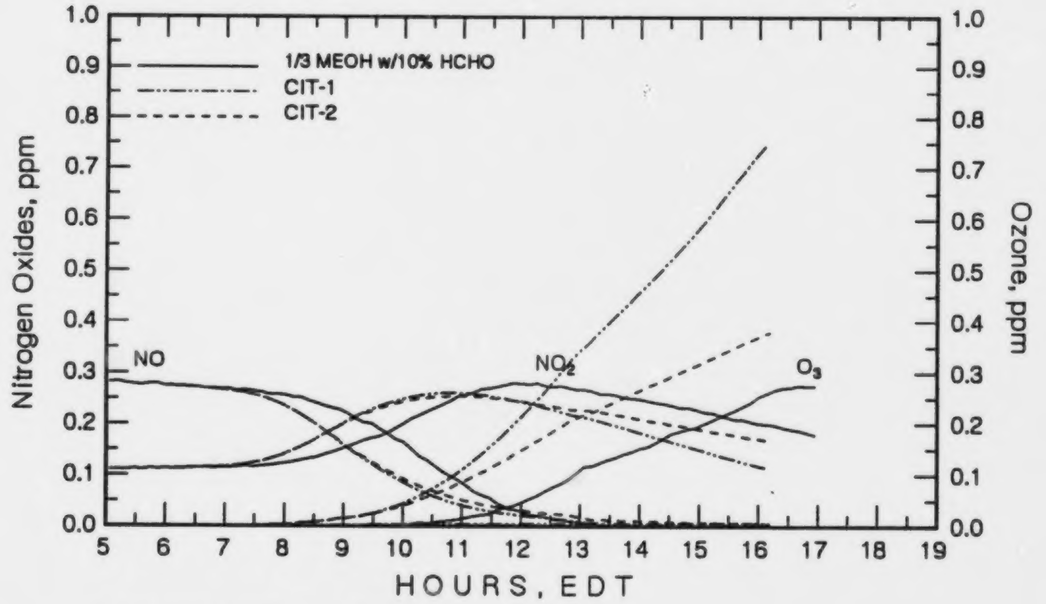


Figure A123. CIT Predictions.

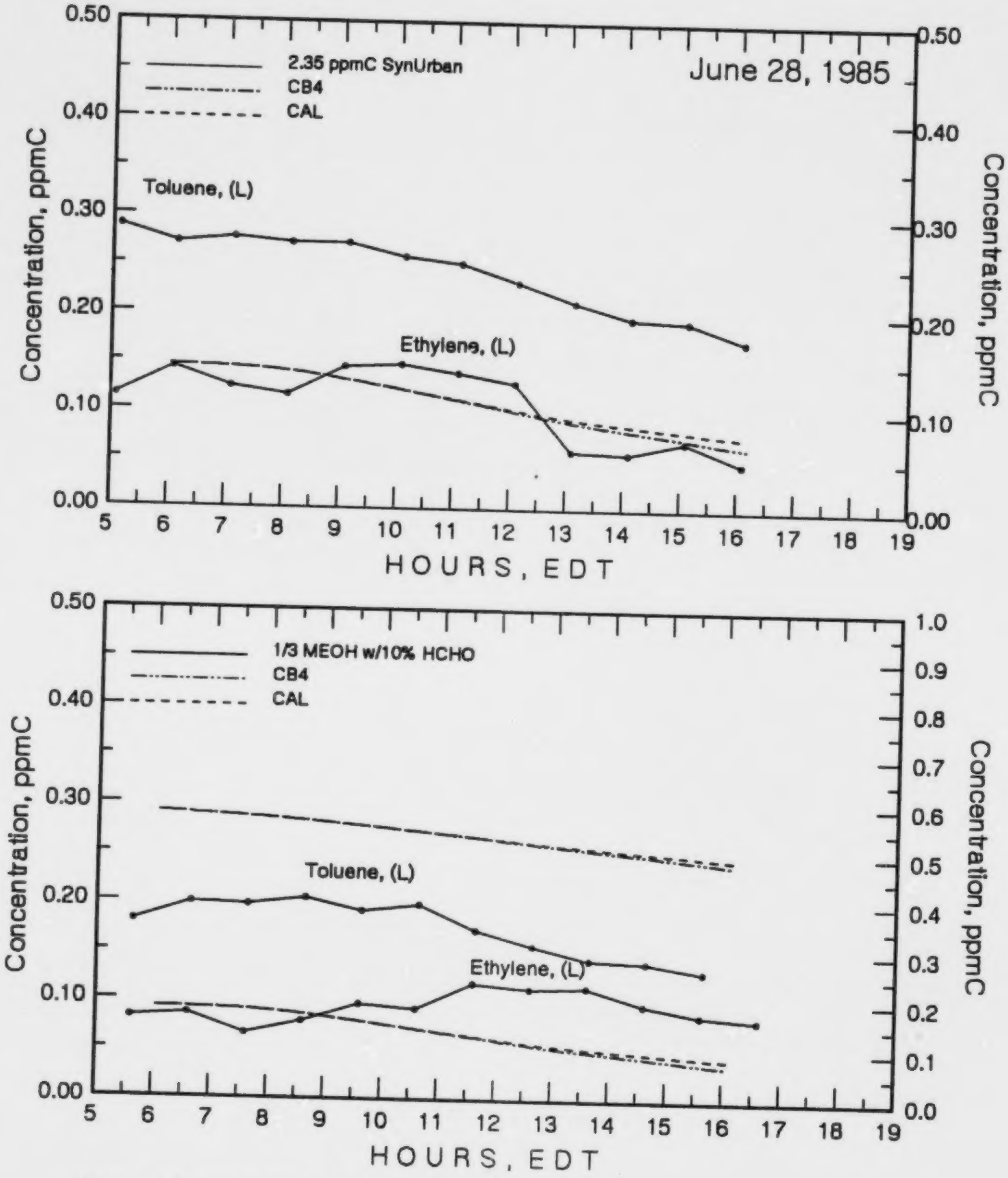


Figure A124. CIT Predicitons.

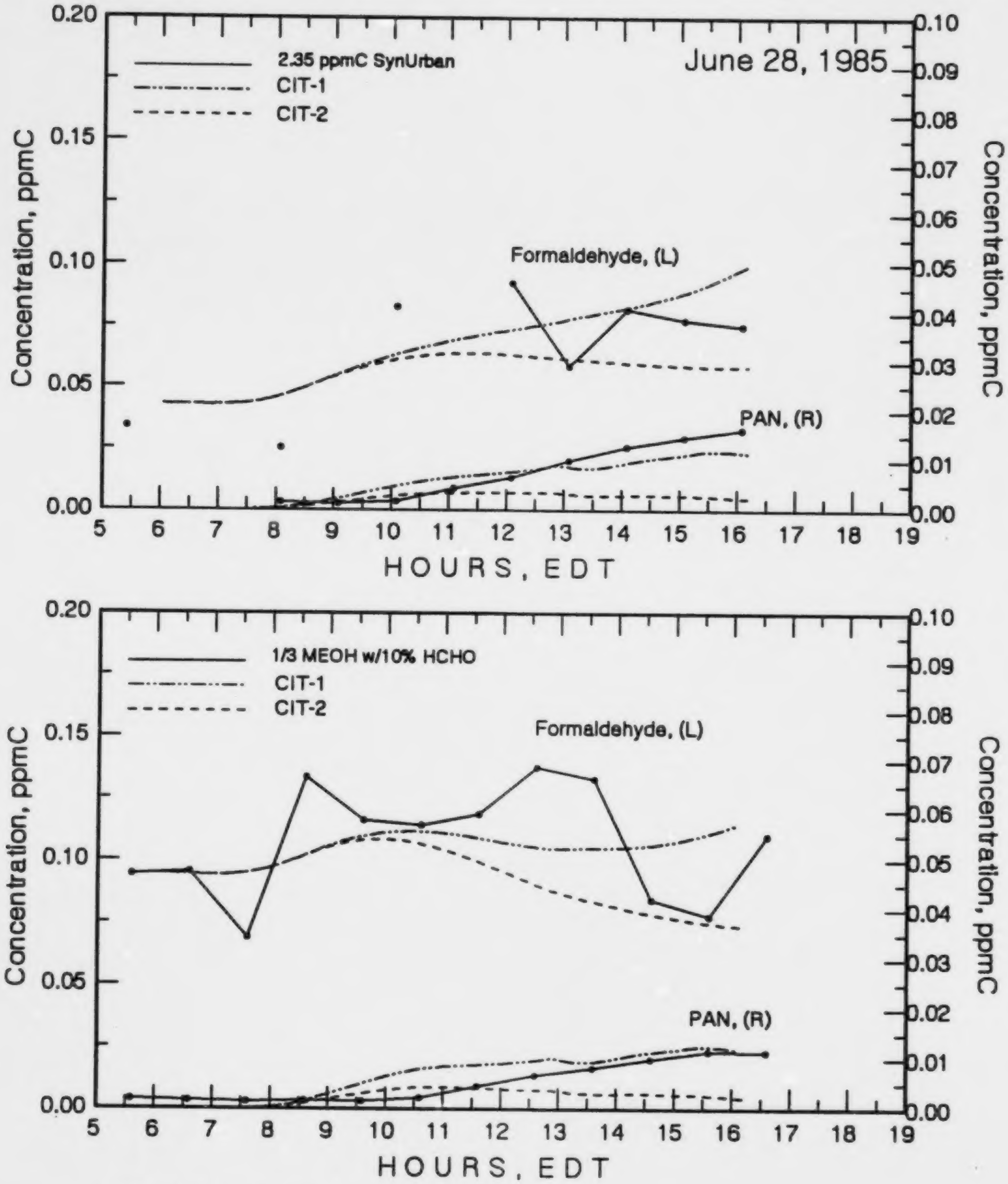


Figure A125. CIT Predictions.

Final
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Methanol Fueled Vehicles and Photochemical Models:

An Evaluation of the State of Knowledge

Appendices B and C

By

Terry Keating

Department of Environmental Sciences and Engineering
School of Public Health
University of North Carolina, Chapel Hill

May, 1989

Sponsored By

The National Network for Environmental Management Studies
U.S. Environmental Protection Agency

B-C-i

Methanol Fueled Vehicles and Photochemical Models:

An Evaluation of the State of Knowledge

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Department of Environmental Sciences and Engineering
School of Public Health
University of North Carolina, Chapel Hill

May, 1989

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U.S. Environmental Protection Agency

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Appendix B

Initial Conditions of Model Simulations

B-C-iv

This appendix contains all of the actual initial condition files used by PKSS-PC to generate the plots in Appendix A. Each set of three plots in Appendix A contains the outputs of two mechanisms for both sides of the chamber. Thus, for each set of three plots in Appendix A, there are four initial condition files.

```
Aug 4, 1984 1.25 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CALCHMw.PKS
CONC=
NO =                    0.291,
NO2 =                   0.077,
ALK4 = 0.0249,
ALK7 = 0.0186,
ETHE = 0.1827,
PRPE = 0.0254,
TBUT = 0.0073,
TOLU = 0.0337,
XYLE = 0.0200,
TMBZ = 0.0069,
HCHO =          0.0189,
      (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0054,
CO    =        0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,TMBZ,
HCHO,
ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (RED DEWPOINT)
  0: 29251.4,  57: 29678.8, 121: 34722.1, 185: 3C483.0, 241:
36879.8,
297: 37525.6, 433: 37201.0, 481: 37771.5, 537: 38143.7, 615:
39072.6;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984  1.25 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CB42CHMw.PKS
CONC=
NO =                    0.291,
NO2 =                   0.077,
PAR  =                  0.2888,
ETH   =                 0.1827,
OLE    =                0.0254,
TOL     =               0.0337,
XYL      =              0.0269,
RCHO      =             0.0146,
HCHO       =            0.0189,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0054,
CO   =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (RED DEWPOINT)
  0: 29251.4,  57: 29678.8, 121: 34722.1, 185: 36483.0, 241:
36879.8,
297: 37525.6, 433: 37201.0, 481: 37771.5, 537: 38143.7, 615:
39072.6;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984 0.82 ppmC SYNAUTO, 0.32 ppm MeOH, 0.041 ppm HCHO
(BLUE)
C:\pkss\MECH\Calchmw.PKS
CONC=
NO    =          0.284,
NO2   =          0.071,
HCHO  =          0.0412,
MEOH  = 0.3209,
ALK4  =          0.0170,
ALK7  =          0.0124,
ETHE  =          0.1220,
PRPE  =          0.0166,
TBUT  =          0.0049,
TOLU  =          0.0221,
XYLE  =          0.0132,
TMBZ  =          0.0045,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.005,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,TMBZ,
HCHO,
ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (AUG 4 1984 BLUE DEWPOINT)
  0:29070.0,   61: 30051.1, 117: 33062.8, 181: 34426.6,   237:
35096.1, 301: 35209.1, 429: 35474.8, 477: 36208.0, 541:
36561.8, 615:37080.2;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984 0.82 ppmC SYNAUTO, 0.32 ppm MeOH, 0.041 ppm HCHO
(BLUE)
C:\PKSS\MECH\CB42CHMw.PKS
CONC=
NO     =           0.284,
NO2    =           0.071,
HCHO   =    0.041,
MEOH   =    0.3209,
RCHO   =    0.0097,
PAR    =    0.1949,
ETH    =    0.1220,
OLE    =    0.0166,
TOL    =    0.0221,
XYL    =    0.0177,
PAR    =    0.0201,
ETH    =    0.0009,
OLE    =    0.0006,
TOL    =    0.0004,
XYL    =    0.0003,
HCHO   =    0.0038,
RCHO   =    0.0030,
HONO   =           0.005,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (AUG 4 1984 BLUE DEWPOINT)
  0:29070.0,   61: 30051.1, 117: 33062.8, 181: 34426.6,   237:
35096.1, 301: 35209.1, 429: 35474.8, 477: 36208.0, 541:
36561.8, 615:37080.2;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984 1.25 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CALCHMK.PKS
CONC=
NO =                  0.291,
NO2 =                 0.077,
ALK4 = 0.0249,
ALK7 = 0.0186,
ETHE = 0.1827,
PRPE = 0.0254,
TBUT = 0.0073,
TOLU = 0.0337,
XYLE = 0.0200,
TMBZ = 0.0069,
HCHO =        0.0189,
        (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0054,
CO    =        0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,TMBZ,
HCHO,
ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
     0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (RED DEWPOINT)
  0: 29251.4,  57: 29678.8, 121: 34722.1, 185: 36483.0, 241:
36879.8,
297: 37525.6, 433: 37201.0, 481: 37771.5, 537: 38143.7, 615:
39072.6;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984  1.25 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CB42CHMK.PKS
CONC=
NO =                    0.291,
NO2 =                   0.077,
PAR  =                  0.2888,
ETH   =                 0.1827,
OLE    =                0.0254,
TOL     =               0.0337,
XYL      =              0.0269,
RCHO      =             0.0146,
HCHO       =            0.0189,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0054,
CO    =        0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,    185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,    537:  312.5,
615:  311.0;
WATER= (RED DEWPOINT)
  0: 29251.4,  57: 29678.8, 121: 34722.1, 185: 36483.0, 241:
36879.8,
297: 37525.6, 433: 37201.0, 481: 37771.5, 537: 38143.7, 615:
39072.6;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984 0.82 ppmC SYNAUTO, 0.32 ppm MeOH, 0.041 ppm HCHO
(BLUE)
C:\PKSS\MECH\CALCHMK.PKS
CONC=
NO     =           0.284,
NO2    =           0.071,
HCHO   =           0.0412,
MEOH   = 0.3209,
ALK4   =           0.0170,
ALK7   =           0.0124,
ETHE   =           0.1220,
PRPE   =           0.0166,
TBUT   =           0.0049,
TOLU   =           0.0221,
XYLE   =           0.0132,
TMBZ   =           0.0045,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =           0.005,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,TMBZ,
HCHO,
ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (AUG 4 1984 BLUE DEWPOINT)
  0:29070.0,   61: 30051.1, 117: 33062.8, 181: 34426.6,   237:
35096.1, 301: 35209.1, 429: 35474.8, 477: 36208.0, 541:
36561.8, 615:37080.2;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984 0.82 ppmC SYNAUTO, 0.32 ppm MeOH, 0.041 ppm HCHO
(BLUE)
C:\PKSS\MECH\CB42CHMK.PKS
CONC=
NO    =          0.284,
NO2   =          0.071,
HCHO  =   0.041,
MEOH  =   0.3209,
RCHO  =   0.0097,
PAR   =   0.1949,
ETH   =   0.1220,
OLE   =   0.0166,
TOL   =   0.0221,
XYL   =   0.0177,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.005,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (AUG 4 1984 BLUE DEWPOINT)
  0:29070.0,   61: 30051.1, 117: 33062.8, 181: 34426.6,   237:
35096.1, 301: 35209.1, 429: 35474.8, 477: 36208.0, 541:
36561.8, 615:37080.2;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984 1.25 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CALCHMN.PKS
CONC=
NO =                   0.291,
NO2 =                  0.077,
ALK4 = 0.0249,
ALK7 = 0.0186,
ETHE = 0.1827,
PRPE = 0.0254,
TBUT = 0.0073,
TOLU = 0.0337,
XYLE = 0.0200,
TMBZ = 0.0069,
HCHO =          0.0189,
      (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0054,
CO    =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,TMBZ,
HCHO,
ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (RED DEWPOINT)
  0: 29251.4, 57: 29678.8, 121: 34722.1, 185: 36483.0, 241:
36879.8,
297: 37525.6, 433: 37201.0, 481: 37771.5, 537: 38143.7, 615:
39072.6;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984  1.25 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CB42CHMN.PKS
CONC=
NO =                  0.291,
NO2 =                 0.077,
PAR  =                0.2888,
ETH   =               0.1827,
OLE    =              0.0254,
TOL     =             0.0337,
XYL      =            0.0269,
RCHO      =           0.0146,
HCHO       =          0.0189,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =          0.0054,
CO    =        0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (RED DEWPOINT)
  0: 29251.4,  57: 29678.8, 121: 34722.1, 185: 36483.0, 241:
36879.8,
297: 37525.6, 433: 37201.0, 481: 37771.5, 537: 38143.7, 615:
39072.6;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984 0.82 ppmC SYNAUTO, 0.32 ppm MeOH, 0.041 ppm HCHO
(BLUE)
C:\PKSS\MECH\CALCHMN.PKS
CONC=
NO    =          0.284,
NO2   =          0.071,
HCHO  =          0.0412,
MEOH  = 0.3209,
ALK4  =          0.0170,
ALK7  =          0.0124,
ETHE  =          0.1220,
PRPE  =          0.0166,
TBUT  =          0.0049,
TOLU  =          0.0221,
XYLE  =          0.0132,
TMBZ  =          0.0045,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.005,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,TMBZ,
HCHO,
ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (AUG 4 1984 BLUE DEWPOINT)
  0:29070.0,   61: 30051.1, 117: 33062.8, 181: 34426.6,   237:
35096.1, 301: 35209.1, 429: 35474.8, 477: 36208.0, 541:
36561.8, 615:37080.2;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 4, 1984 0.82 ppmC SYNAUTO, 0.32 ppm MeOH, 0.041 ppm HCHO
(BLUE)
C:\PKSS\MECH\CB42CHMN.PKS
CONC=
NO     =            0.284,
NO2    =            0.071,
HCHO   =    0.041,
MEOH   =    0.3209,
RCHO   =    0.0097,
PAR    =    0.1949,
ETH    =    0.1220,
OLE    =    0.0166,
TOL    =    0.0221,
XYL    =    0.0177,
PAR    =    0.0201,
ETH    =    0.0009,
OLE    =    0.0006,
TOL    =    0.0004,
XYL    =    0.0003,
HCHO   =    0.0038,
RCHO   =    0.0030,
HONO   =            0.005,
CO     =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0484.LIX;
TEMPERATURE= (August 4, 1984)
    0:  296.2,    57:  296.5,   121:  300.4,   185:  308.5,
241:  308.3,
  297:  309.5,   433:  311.5,   481:  310.5,   537:  312.5,
615:  311.0;
WATER= (AUG 4 1984 BLUE DEWPOINT)
  0:29070.0,   61: 30051.1, 117: 33062.8, 181: 34426.6,   237:
35096.1, 301: 35209.1, 429: 35474.8, 477: 36208.0, 541:
36561.8, 615:37080.2;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 5, 1984 0.9 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO =                   0.272,
NO2 =                  0.079,
ALK4 = 0.0201,
ALK7 = 0.0144,
ETHE  =                0.1326,
PRPE  =                0.0195,
TBUT  =                0.0053,
TOLU    =              0.0246,
XYLE      =            0.0145,
TMBZ =                 0.00502,
HCHO       =           0.0124,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0055,
CO   =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR:C:\PKSS\LIX\AU0584.LIX;
TEMPERATURE=   (AUGUST 5, 1984)
   0 : 295.1 ,   60 : 295.1 ,  120 : 298.8 ,  180 : 302.6 ,
240 : 307.3 ,
 300 : 308.8 ,  360 : 310.8 ,  420 : 311.2 ,  480 : 311.1 ,
540 : 311.3 ,
 610 : 310.8 ;
WATER= (RED AUG 5 84)
    0: 28069.7,  64: 33664.7, 120: 40742.5, 176: 45934.1, 184:
47315.5,
  240: 51235.9, 296: 50002.0, 304: 49771.1, 360: 49828.8, 416:
48636.0,
  424: 48080.4, 480: 48357.2, 536: 48190.9, 544: 47423.9, 610:
48301.6;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 5, 1984 0.9 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO =                0.272,
NO2 =               0.079,
PAR  =              0.2269,
ETH   =             0.1326,
OLE    =            0.0195,
TOL     =           0.0246,
XYL      =          0.0195,
RCHO      =         0.0105,
HCHO       =        0.0124,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =         0.0055,
CO   =        0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR:C:\PKSS\LIX\AU0584.LIX;
TEMPERATURE=   (AUGUST 5, 1984)
   0 : 295.1 ,   60 : 295.1 ,  120 : 298.8 ,  180 : 302.6 ,
240 : 307.3 ,
 300 : 308.8 ,  360 : 310.8 ,  420 : 311.2 ,  480 : 311.1 ,
540 : 311.3 ,
 610 : 310.8 ;
WATER= (RED AUG 5 84)
    0: 28069.7,  64: 33664.7, 120: 40742.5, 176: 45934.1, 184:
47315.5,
  240: 51235.9, 296: 50002.0, 304: 49771.1, 360: 49828.8, 416:
48636.0,
  424: 48080.4, 480: 48357.2, 536: 48190.9, 544: 47423.9, 610:
48301.6;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
Aug 5, 1984 1.3 ppmC SYNAUTO (BLUE)
C:\pkss\MECH\CalchmW.PKS
CONC=
NO     =           0.268,
NO2    =           0.077,
HCHO   =           0.0188,
ALK4   =           0.0293,
ALK7   =           0.0197,
ETHE   =           0.1946,
PRPE   =           0.0290,
TBUT   =           0.0078,
TOLU   =           0.0345,
XYLE   =           0.0210,
TMBZ   =           0.00705,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =           0.0054,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR:C:\PKSS\LIX\AU0584.LIX;
TEMPERATURE=   (AUGUST 5, 1984)
   0 : 295.1 ,   60 : 295.1 ,  120 : 298.8 ,  180 : 302.6 ,
240 : 307.3 ,
 300 : 308.8 ,  360 : 310.8 ,  420 : 311.2 ,  480 : 311.1 ,
540 : 311.3 ,
 610 : 310.8 ;
WATER= (BLUE AUG 5 1984)
    0: 28920.7,  60: 31006.3, 116: 39765.5, 124: 40073.2,
180: 43805.3,
  236: 46459.6,
  244: 47970.3, 300: 45159.7, 356: 45622.3, 364: 45364.5,
420: 43462.3,
  476: 42452.8, 484: 43026.1, 540: 44301.0, 596: 42881.9,
614: 42786.1;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 5, 1984 1.3 ppmC SYNAUTO (BLUE)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO     =          0.268,
NO2    =          0.077,
HCHO   =          0.0188,
RCHO   =          0.0155,
PAR    =          0.3214,
ETH    =          0.1946,
OLE    =          0.0290,
TOL    =          0.0345,
XYL    =          0.0281,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =          0.0054,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR:C:\PKSS\LIX\AU0584.LIX;
TEMPERATURE=   (AUGUST 5, 1984)
   0 : 295.1 ,   60 : 295.1 ,  120 : 298.8 ,  180 : 302.6 ,
240 : 307.3 ,
 300 : 308.8 ,  360 : 310.8 ,  420 : 311.2 ,  480 : 311.1 ,
540 : 311.3 ,
 610 : 310.8 ;
WATER= (BLUE AUG 5 1984)
    0: 28920.7,  60: 31006.3, 116: 39765.5, 124: 40073.2,
180: 43805.3,
  236: 46459.6,
  244: 47970.3, 300: 45159.7, 356: 45622.3, 364: 45364.5,
420: 43462.3,
  476: 42452.8, 484: 43026.1, 540: 44301.0, 596: 42881.9,
614: 42786.1;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 6, 1984 2.3 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO2       =       0.072,
NO        =       0.279,
ETHE    =         0.3330 ,
PRPE    =         0.0493 ,
TBUT    =         0.0130 ,
ALK4    =         0.0502 ,
ALK7    =         0.0325 ,
TOLU    =         0.0602 ,
XYLE    =         0.0366 ,
TMBZ    =         0.0128 ,
HCHO    =         0.0390 ,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO      =       0.005,
CO        =       0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR:C:\PKSS\LIX\AU0684.LIX;
TEMPERATURE= (AUGUST 6, 1984)
   0: 295.2,  62: 295.6,  94: 297.2, 142: 300.5, 182: 303.8,
238: 307.4,
 302: 309.3, 358: 310.7, 422: 312.4, 478: 311.4, 542: 312.9,
614: 312.2;
WATER= (RED)    (AUGUST 6, 1984)
   0: 27697.9,  62:   29556, 118: 33700.5, 182: 36680.7, 238:
37241.4,
 302: 38268.7, 358:   38227, 422:   39985, 486: 42216.6, 542:
42642.8,
 614: 44052.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 6, 1984 2.3 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO2        =        0.072,
NO         =        0.279,
HCHO       =        0.039,
RCHO       =        0.0260,
PAR        =        0.5434,
ETH        =        0.3330,
OLE        =        0.0493,
TOL        =        0.0602,
XYL        =        0.0494,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =           0.005,
CO         =       0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR:C:\PKSS\LIX\AU0684.LIX;
TEMPERATURE= (AUGUST 6, 1984)
   0: 295.2,  62: 295.6,  94: 297.2, 142: 300.5, 182: 303.8,
238: 307.4,
 302: 309.3, 358: 310.7, 422: 312.4, 478: 311.4, 542: 312.9,
614: 312.2;
WATER= (RED)    (AUGUST 6, 1984)
   0: 27697.9,  62:   29556, 118: 33700.5, 182: 36680.7, 238:
37241.4,
 302: 38268.7, 358:   38227, 422:   39985, 486: 42216.6, 542:
42642.8,
 614: 44052.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 6, 1984 3.3 ppmC SYNAUTO (BLUE)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO     =            0.283,
NO2    =            0.072,
ETHE     =          0.4813 ,
PRPE     =          0.0710 ,
TBUT     =          0.0197 ,
ALK4     =          0.0711 ,
ALK7     =          0.0481 ,
TOLU     =          0.0860 ,
XYLE     =          0.0520 ,
TMBZ     =          0.0180 ,
HCHO     =          0.0570 ,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =          0.005,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR:C:\PKSS\LIX\AU0684.LIX;
TEMPERATURE= (AUGUST 6, 1984)
   0: 295.2,  62: 295.6,  94: 297.2, 142: 300.5, 182: 303.8,
238: 307.4,
 302: 309.3, 358: 310.7, 422: 312.4, 478: 311.4, 542: 312.9,
614: 312.2;
WATER= (BLUE AUGUST 6, 1984)
   0: 27926.1,  58: 28831.3, 122: 32888.1, 178: 34983.4, 242:
35858.5,
 298: 36720.4, 362: 36999.8, 426: 37812.5, 482: 40161.7, 546:
40697.6,
 610:   42834;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
August 6, 1984 3.3 ppmC SYNAUTO (BLUE)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO     =          0.283,
NO2    =          0.072,
HCHO   =          0.057,
RCHO   =          0.0395,
PAR    =          0.7879,
ETH    =          0.4813,
OLE    =          0.0710,
TOL    =          0.0860,
XYL    =          0.0700,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =          0.005,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR:C:\PKSS\LIX\AU0684.LIX;
TEMPERATURE= (AUGUST 6, 1984)
   0: 295.2,  62: 295.6,  94: 297.2, 142: 300.5, 182: 303.8,
238: 307.4,
 302: 309.3, 358: 310.7, 422: 312.4, 478: 311.4, 542: 312.9,
614: 312.2;
WATER= (BLUE AUGUST 6, 1984)
   0: 27926.1,  58: 28831.3, 122: 32888.1, 178: 34983.4, 242:
35858.5,
 298: 36720.4, 362: 36999.8, 426: 37812.5, 482: 40161.7, 546:
40697.6,
 610:   42834;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 7, 1984 1.36 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO =                   0.302,
NO2 =                  0.083,
ALK4 = 0.0289,
ALK7 = 0.0204,
ETHE = 0.1906,
PRPE = 0.0273,
TBUT = 0.0072,
TOLU = 0.0356,
XYLE = 0.0217,
TMBZ = 0.0073,
HCHO =        0.0411,
      (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0058,
CO    =        0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0784.LIX;
TEMPERATURE= (AUG 7 84)
    0:  296.2,    62:  296.6,   118:  300.3,   126:  301.2,
  182:  305.3,   238:  308.1,   246:  308.4,   294:  309.5,
  358:  311.4,   366:  311.6,   414:  312.9,   422:  312.9,
  478:  312.5,   486:  312.5,   542:  311.8,   616:  311.3;
WATER= (RED AUG 7 1984)
    0: 29926.0,   126: 32302.8,   174: 35360.7,   182:
35627.7,   238: 36325.6,   246: 36052.2,   294: 35858.5,
  302: 36919.7,   358: 37895.0,   366: 37120.4,   414:
38102.2,   422: 37689.2,
  478: 39590.8,   486: 40117.4,   534: 38604.8,   542:
37403.5,   616: 39158.3;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 7, 1984  1.36 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO =                  0.302,
NO2 =                 0.083,
PAR  =                0.3214,
ETH   =               0.1906,
OLE    =              0.0273,
TOL     =             0.0356,
XYL      =            0.0290,
RCHO      =           0.0144,
HCHO       =          0.0411,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =         0.0058,
CO   =        0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0784.LIX;
TEMPERATURE= (AUG 7 84)
    0:  296.2,    62:  296.6,   118:  300.3,   126:  301.2,
  182:  305.3,   238:  308.1,   246:  308.4,   294:  309.5,
  358:  311.4,   366:  311.6,   414:  312.9,   422:  312.9,
  478:  312.5,   486:  312.5,   542:  311.8,   616:  311.3;
WATER= (RED AUG 7 1984)
    0: 29926.0,   126: 32302.8,   174: 35360.7,   182:
35627.7,   238: 36325.6,   246: 36052.2,   294: 35858.5,
  302: 36919.7,   358: 37895.0,   366: 37120.4,   414:
38102.2,   422: 37689.2,
  478: 39590.8,   486: 40117.4,   534: 38604.8,   542:
37403.5,   616: 39158.3;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 7, 1984 0.87 ppmC SYNAUTO, 0.30 ppm MeOH, 0.056 ppm HCHO
(BLUE)
C:\pkss\MECH\CalchmW.PKS
CONC=
NO     =            0.296,
NO2    =            0.084,
HCHO   =            0.0555,
MEOH   = 0.3209,
ALK4   =            0.0194,
ALK7   =            0.0140,
ETHE   =            0.1255,
PRPE   =            0.0182,
TBUT   =            0.0051,
TOLU   =            0.0221,
XYLE   =            0.0142,
TMBZ   =            0.0045,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =  0.0038,
ALD2   =  0.0030,
HONO   =            0.0059,
CO     =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0784.LIX;
TEMPERATURE= (AUG 7 84)
    0:  296.2,    62:  296.6,   118:  300.3,   126:  301.2,
  182:  305.3,   238:  308.1,   246:  308.4,   294:  309.5,
  358:  311.4,   366:  311.6,   414:  312.9,   422:  312.9,
  478:  312.5,   486:  312.5,   542:  311.8,   616:  311.3;
WATER= (BLUE AUG 7 84)
    0: 30207.8,   122: 30397.2,   178: 33238.5,   242:
33450.7,   298: 33593.2,
  306: 33808.2,   354: 34463.3,   362: 35398.7,   418:
35058.5,   426: 35820.0,
  474: 36404.2,   482: 37040.0,   538: 35247.0,   546:
35589.4,   612: 36760.1;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
Aug 7, 1984 0.87 ppmC SYNAUTO, 0.30 ppm MeOH, 0.056 ppm HCHO
(BLUE)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO     =            0.296,
NO2    =            0.084,
HCHO   =   0.0555,
MEOH   =   0.2987,
RCHO   =   0.0102,
PAR    =   0.2180,
ETH    =   0.1255,
OLE    =   0.0182,
TOL    =   0.0221,
XYL    =   0.0187,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =            0.0059,
CO     =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0784.LIX;
TEMPERATURE= (AUG 7 84)
    0:  296.2,    62:  296.6,   118:  300.3,   126:  301.2,
  182:  305.3,   238:  308.1,   246:  308.4,   294:  309.5,
  358:  311.4,   366:  311.6,   414:  312.9,   422:  312.9,
  478:  312.5,   486:  312.5,   542:  311.8,   616:  311.3;
WATER= (BLUE AUG 7 84)
    0: 30207.8,   122: 30397.2,   178: 33238.5,   242:
33450.7,   298: 33593.2,
  306: 33808.2,   354: 34463.3,   362: 35398.7,   418:
35058.5,   426: 35820.0,
  474: 36404.2,   482: 37040.0,   538: 35247.0,   546:
35589.4,   612: 36760.1;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 7, 1984 1.36 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO =                    0.302,
NO2 =                   0.083,
ALK4 = 0.0289,
ALK7 = 0.0204,
ETHE = 0.1906,
PRPE = 0.0273,
TBUT = 0.0072,
TOLU = 0.0356,
XYLE = 0.0217,
TMBZ = 0.0073,
HCHO =          0.0411,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =            0.0058,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0784.LIX;
TEMPERATURE= (AUG 7 84)
    0:  296.2,    62:  296.6,   118:  300.3,   126:  301.2,
  182:  305.3,   238:  308.1,   246:  308.4,   294:  309.5,
  358:  311.4,   366:  311.6,   414:  312.9,   422:  312.9,
  478:  312.5,   486:  312.5,   542:  311.8,   616:  311.3;
WATER= (RED AUG 7 1984)
    0: 29926.0,   126: 32302.8,   174: 35360.7,   182:
35627.7,   238: 36325.6,   246: 36052.2,   294: 35858.5,
  302: 36919.7,   358: 37895.0,   366: 37120.4,   414:
38102.2,   422: 37689.2,
  478: 39590.8,   486: 40117.4,   534: 38604.8,   542:
37403.5,   616: 39158.3;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
Aug 7, 1984  1.36 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO =                 0.302,
NO2 =                0.083,
PAR  =               0.3214,
ETH   =              0.1906,
OLE    =             0.0273,
TOL     =            0.0356,
XYL      =           0.0290,
RCHO      =          0.0144,
HCHO       =         0.0411,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0058,
CO   =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0784.LIX;
TEMPERATURE= (AUG 7 84)
    0:  296.2,    62:  296.6,   118:  300.3,   126:  301.2,
  182:  305.3,   238:  308.1,   246:  308.4,   294:  309.5,
  358:  311.4,   366:  311.6,   414:  312.9,   422:  312.9,
  478:  312.5,   486:  312.5,   542:  311.8,   616:  311.3;
WATER= (RED AUG 7 1984)
    0: 29926.0,   126: 32302.8,   174: 35360.7,   182:
35627.7,   238: 36325.6,   246: 36052.2,   294: 35858.5,
  302: 36919.7,   358: 37895.0,   366: 37120.4,   414:
38102.2,   422: 37689.2,
  478: 39590.8,   486: 40117.4,   534: 38604.8,   542:
37403.5,   616: 39158.3;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 7, 1984 0.87 ppmC SYNAUTO, 0.30 ppm MeOH, 0.056 ppm HCHO
(BLUE)
C:\pkss\MECH\CalchmW.PKS
CONC=
NO    =            0.296,
NO2   =            0.084,
HCHO  =            0.0555,
MEOH  = 0.3209,
MEONO = 0.003,
ALK4  =            0.0194,
ALK7  =            0.0140,
ETHE  =            0.1255,
PRPE  =            0.0182,
TBUT  =            0.0051,
TOLU  =            0.0221,
XYLE  =            0.0142,
TMBZ  =            0.0045,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =            0.0059,
CO    =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0784.LIX;
TEMPERATURE= (AUG 7 84)
    0:  296.2,   62:  296.6,   118:  300.3,   126:  301.2,
  182:  305.3,  238:  308.1,   246:  308.4,   294:  309.5,
  358:  311.4,  366:  311.6,   414:  312.9,   422:  312.9,
  478:  312.5,  486:  312.5,   542:  311.8,   616:  311.3;
WATER= (BLUE AUG 7 84)
    0: 30207.8,   122: 30397.2,   178: 33238.5,   242:
33450.7,   298: 33593.2,
  306: 33808.2,   354: 34463.3,   362: 35398.7,   418:
35058.5,   426: 35820.0,
  474: 36404.2,   482: 37040.0,   538: 35247.0,   546:
35589.4,   612: 36760.1;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
Aug 7, 1984 0.87 ppmC SYNAUTO, 0.30 ppm MeOH, 0.056 ppm HCHO
(BLUE)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO    =           0.296,
NO2   =           0.084,
HCHO  =   0.0555,
MEOH  =   0.2987,
MEONO =   0.003,
RCHO  =   0.0102,
PAR   =   0.2180,
ETH   =   0.1255,
OLE   =   0.0182,
TOL   =   0.0221,
XYL   =   0.0187,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =           0.0059,
CO    =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0784.LIX;
TEMPERATURE= (AUG 7 84)
    0:  296.2,    62:  296.6,   118:  300.3,   126:  301.2,
  182:  305.3,   238:  308.1,   246:  308.4,   294:  309.5,
  358:  311.4,   366:  311.6,   414:  312.9,   422:  312.9,
  478:  312.5,   486:  312.5,   542:  311.8,   616:  311.3;
WATER= (BLUE AUG 7 84)
    0: 30207.8,   122: 30397.2,   178: 33238.5,   242:
33450.7,   298: 33593.2,
  306: 33808.2,   354: 34463.3,   362: 35398.7,   418:
35058.5,   426: 35820.0,
  474: 36404.2,   482: 37040.0,   538: 35247.0,   546:
35589.4,   612: 36760.1;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 8, 1984 2.5 ppmC SYNAUTO, 0.79 ppm MeOH, 0.23 ppm HCHO
(RED)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO    =           0.262,
NO2   =           0.076,
ETHE    =         0.3525 ,
PRPE    =         0.0521 ,
TBUT    =         0.0145 ,
ALK4    =         0.0525 ,
ALK7    =         0.0388 ,
TOLU    =         0.0687 ,
XYLE    =         0.0407 ,
TMBZ    =         0.0140 ,
HCHO    =         0.228,
MEOH    =         0.795,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =          0.0053,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR:C:\PKSS\LIX\AU0884.LIX;
TEMPERATURE= (AUG 8 88)
    0:  295.4,    61:  295.8,   117:  299.3,   181:  303.4,
  237:  307.0,   245:  307.5,   301:  309.4,   357:  311.1,
  421:  311.5,   485:  311.6,   541:  312.2,   615:  311.2;
WATER= (RED AUG 8 88)
    0: 27669.6,    61: 29988.7,   117: 28831.3,   181:
29648.1,
  237: 30333.9,   245: 30333.9,   301: 30333.9,   357:
30716.0,
  421: 31530.6,   477: 32302.8,   541: 32302.8,   615:
33379.8;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 8, 1984 2.5 ppmC SYNAUTO, 0.79 ppm MeOH, 0.23 ppm HCHO
(RED)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO     =           0.262,
NO2    =           0.076,
ETH      =         0.3525 ,
OLE      =         0.0521 ,
PAR      =         0.6038 ,
TOL      =         0.0687 ,
XYL      =         0.0547 ,
MEOH     =         0.7950,
HCHO     =         0.228,
RCHO     =         0.0289 ,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =           0.0053,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=c:\pkss\lix\AU0884.LIX;
TEMPERATURE= (AUG 8 88)
    0:  295.4,    61:  295.8,   117:  299.3,   181:  303.4,
  237:  307.0,   245:  307.5,   301:  309.4,   357:  311.1,
  421:  311.5,   485:  311.6,   541:  312.2,   615:  311.2;
WATER= (RED AUG 8 88)
    0: 27669.6,    61: 29988.7,   117: 28831.3,   181:
29648.1,
  237: 30333.9,   245: 30333.9,   301: 30333.9,   357:
30716.0,
  421: 31530.6,   477: 32302.8,   541: 32302.8,   615:
33379.8;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 8, 1984 2.5 ppmC SYNAUTO, 0.79 ppm MeOH, 0.23 ppm HCHO
(RED)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO    =           0.262,
NO2   =           0.076,
ETH     =         0.3525 ,
OLE     =         0.0521 ,
PAR     =         0.6038 ,
TOL     =         0.0687 ,
XYL     =         0.0547 ,
MEOH    =         0.7950,
HCHO    =         0.228,
RCHO    =         0.0289 ,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0053,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=c:\pkss\lix\AU0884.LIX;
TEMPERATURE= (AUG 8 88)
    0:  295.4,    61:  295.8,   117:  299.3,   181:  303.4,
  237:  307.0,   245:  307.5,   301:  309.4,   357:  311.1,
  421:  311.5,   485:  311.6,   541:  312.2,   615:  311.2;
WATER= (RED AUG 8 88)
    0: 27669.6,    61: 29988.7,   117: 28831.3,   181:
29648.1,
  237: 30333.9,   245: 30333.9,   301: 30333.9,   357:
30716.0,
  421: 31530.6,   477: 32302.8,   541: 32302.8,   615:
33379.8;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 8, 1984 3.7 ppmC SYNAUTO (BLUE)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO     =           0.265,
NO2    =           0.075,
ETHE      =        0.5252 ,
PRPE      =        0.0763 ,
TBUT      =        0.0223 ,
ALK4      =        0.0779 ,
ALK7      =        0.0569 ,
TOLU      =        0.1021 ,
XYLE      =        0.0594 ,
TMBZ      =        0.0209 ,
HCHO      =        0.0570 ,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =           0.0053,
CO    =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR:C:\PKSS\LIX\AU0884.LIX;
TEMPERATURE= (AUG 8 88)
    0:  295.4,    61:  295.8,    117:  299.3,    181:  303.4,
  237:  307.0,   245:  307.5,    301:  309.4,    357:  311.1,
  421:  311.5,   485:  311.6,    541:  312.2,    615:  311.2;
WATER= (BLUE AUG 8 88)
    0: 29525.3,    57: 29464.2,    121: 27783.2,    177:
28742.1,
  241: 29010.4,   297: 29251.4,    305: 29494.8,    361:
29342.4,
  417: 30302.4,   481: 31563.6,    537: 31234.4,    610:
32133.0;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
August 8, 1984 3.7 ppmC SYNAUTO (BLUE)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO    =          0.265,
NO2   =          0.075,
ETH     =        0.5252 ,
OLE     =        0.0763 ,
PAR     =        0.8888 ,
TOL     =        0.1021 ,
XYL     =        0.0803 ,
HCHO    =        0.0570 ,
RCHO    =        0.0445 ,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0053,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0884.LIX;
TEMPERATURE= (AUG 8 88)
    0:  295.4,    61:  295.8,   117:  299.3,   181:  303.4,
  237:  307.0,   245:  307.5,   301:  309.4,   357:  311.1,
  421:  311.5,   485:  311.6,   541:  312.2,   615:  311.2;
WATER= (BLUE AUG 8 88)
    0: 29525.3,    57: 29464.2,   121: 27783.2,   177:
28742.1,
  241: 29010.4,   297: 29251.4,   305: 29494.8,   361:
29342.4,
  417: 30302.4,   481: 31563.6,   537: 31234.4,   610:
32133.0;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 8, 1984 2.5 ppmC SYNAUTO, 0.79 ppm MeOH, 0.23 ppm HCHO
(RED)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO    =          0.262,
NO2   =          0.076,
ETHE     =       0.3523 ,
PRPE     =       0.0521 ,
TBUT     =       0.0145 ,
ALK4     =       0.0524 ,
ALK7     =       0.0388 ,
TOLU     =       0.0686 ,
XYLE     =       0.0401 ,
TMBZ     =       0.0140 ,
HCHO     =       0.228,
MEOH     =       0.785,
MEONO    =       0.010,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0053,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR:C:\PKSS\LIX\AU0884.LIX;
TEMPERATURE= (AUG 8 88)
    0:  295.4,    61:  295.8,   117:  299.3,    181:  303.4,
  237:  307.0,   245:  307.5,   301:  309.4,    357:  311.1,
  421:  311.5,   485:  311.6,   541:  312.2,    615:  311.2;
WATER= (RED AUG 8 88)
    0: 27669.6,    61: 29988.7,    117: 28831.3,    181:
29648.1,
  237: 30333.9,   245: 30333.9,    301: 30333.9,    357:
30716.0,
  421: 31530.6,   477: 32302.8,    541: 32302.8,    615:
33379.8;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
August 8, 1984 2.5 ppmC SYNAUTO, 0.79 ppm MeOH, 0.23 ppm HCHO
(RED)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO     =          0.262,
NO2    =          0.076,
ETH      =        0.3523 ,
OLE      =        0.0521 ,
PAR      =        1.3884 ,
TOL      =        0.0686 ,
XYL      =        0.0541 ,
MEOH     =        0.7850,
MEONO    =        0.010,
HCHO     =        0.228,
RCHO     =        0.0289 ,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =          0.0053,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=c:\pkss\lix\AU0884.LIX;
TEMPERATURE= (AUG 8 88)
    0:  295.4,    61:  295.8,   117:  299.3,   181:  303.4,
  237:  307.0,   245:  307.5,   301:  309.4,   357:  311.1,
  421:  311.5,   485:  311.6,   541:  312.2,   615:  311.2;
WATER= (RED AUG 8 88)
    0: 27669.6,    61: 29988.7,   117: 28831.3,   181:
29648.1,
  237: 30333.9,   245: 30333.9,   301: 30333.9,   357:
30716.0,
  421: 31530.6,   477: 32302.8,   541: 32302.8,   615:
33379.8;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 8, 1984 3.7 ppmC SYNAUTO (BLUE)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO    =          0.265,
NO2   =          0.075,
ETHE    =        0.5252 ,
PRPE    =        0.0763 ,
TBUT    =        0.0223 ,
ALK4    =        0.0779 ,
ALK7    =        0.0569 ,
TOLU    =        0.1021 ,
XYLE    =        0.0594 ,
TMBZ    =        0.0209 ,
HCHO    =        0.0570 ,
      (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0053,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR:C:\PKSS\LIX\AU0884.LIX;
TEMPERATURE= (AUG 8 88)
    0:  295.4,    61:  295.8,    117:  299.3,    181:  303.4,
  237:  307.0,   245:  307.5,    301:  309.4,    357:  311.1,
  421:  311.5,   485:  311.6,    541:  312.2,    615:  311.2;
WATER= (BLUE AUG 8 88)
    0: 29525.3,    57: 29464.2,    121: 27783.2,    177:
28742.1,
  241: 29010.4,   297: 29251.4,    305: 29494.8,    361:
29342.4,
  417: 30302.4,   481: 31563.6,    537: 31234.4,    610:
32133.0;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 8, 1984 3.7 ppmC SYNAUTO (BLUE)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO    =          0.265,
NO2   =          0.075,
ETH     =        0.5252 ,
OLE     =        0.0763 ,
PAR     =        0.8888 ,
TOL     =        0.1021 ,
XYL     =        0.0803 ,
HCHO    =        0.0570 ,
RCHO    =        0.0445 ,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0053,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0884.LIX;
TEMPERATURE= (AUG 8 88)
    0:  295.4,    61:  295.8,    117:  299.3,    181:  303.4,
  237:  307.0,   245:  307.5,    301:  309.4,    357:  311.1,
  421:  311.5,   485:  311.6,    541:  312.2,    615:  311.2;
WATER= (BLUE AUG 8 88)
    0: 29525.3,    57: 29464.2,   121: 27783.2,   177:
28742.1,
  241: 29010.4,   297: 29251.4,   305: 29494.8,   361:
29342.4,
  417: 30302.4,   481: 31563.6,   537: 31234.4,   610:
32133.0;
DILUTION=
  0: 1.5E-4,
610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 9, 1984 1.30 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO =   0.302,
NO2 =  0.087,
ALK4 = 0.0269,
ALK7 = 0.0213,
ETHE = 0.1726,
PRPE = 0.0266,
TBUT = 0.0073,
TOLU = 0.0366,
XYLE = 0.0214,
TMBZ = 0.0075,
HCHO = 0.0188,
        (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0061,
CO   =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0984.LIX;
TEMPERATURE= (AUG 9 88)
    0:  296.2,    61:  296.7,    117:  299.3,   181:  303.6,
  237:  307.9,   301:  310.5,    357:  312.5,   365:  312.5,
  421:  313.1,   477:  313.5,    485:  313.3,   615:313.8;
WATER= (RED AUG 9 88)
    0: 29342.4,    61: 30492.4,   117: 33238.5,   181:
32888.1,
  237: 33203.2,   245: 32853.4,   301: 33309.0,   357:
33664.7,
  421: 34463.3,   477: 34722.1,   485: 34206.8,   615:
34722.0;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
Aug 9, 1984  1.30 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO =                    0.302,
NO2 =                   0.088,
PAR  =                  0.3200,
ETH   =                 0.1726,
OLE    =                0.0266,
TOL     =               0.0366,
XYL      =              0.0288,
RCHO      =             0.0146,
HCHO       =            0.0188,
(background)
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0061,
CO    =        0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0984.LIX;
TEMPERATURE= (AUG 9 88)
    0:  296.2,    61:  296.7,    117:  299.3,    181:  303.6,
  237:  307.9,   301:  310.5,    357:  312.5,    365:  312.5,
  421:  313.1,   477:  313.5,    485:  313.3,    615:313.8;
WATER= (RED AUG 9 88)
    0: 29342.4,    61: 30492.4,    117: 33238.5,    181:
32888.1,
  237: 33203.2,   245: 32853.4,    301: 33309.0,    357:
33664.7,
  421: 34463.3,   477: 34722.1,    485: 34206.8,    615:
34722.0;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
Aug 9, 1984 0.86 ppmC SYNAUTO, 0.26 ppm MeOH, 0.076 ppm HCHO
(BLUE)
C:\pkss\MECH\CalchmW.PKS
CONC=
NO    =          0.298,
NO2   =          0.089,
HCHO  =          0.0763,
MEOH  =          0.2649,
ALK4  =          0.0186,
ALK7  =          0.0145,
ETHE  =          0.1255,
PRPE  =          0.0179,
TBUT  =          0.0048,
TOLU  =          0.0235,
XYLE  =          0.0139,
TMBZ  =          0.0048,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0062,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0984.LIX;
TEMPERATURE= (AUG 9 88)
    0:  296.2,    61:  296.7,    117:  299.3,    181:  303.6,
  237:  307.9,   301:  310.5,    357:  312.5,    365:  312.5,
  421:  313.1,   477:  313.5,    485:  313.3,    615:313.8;
WATER= (BLUE AUG 9 88)
    0: 29190.9,    57: 29988.7,    121: 32302.8,    177:
31071.3,
  185: 31530.6,   241: 31234.4,    297: 32065.3,    361:
32784.0,
  417: 33415.3,   481: 33273.7,    537: 32957.9,    615:
34061.0;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 9, 1984 0.86 ppmC SYNAUTO, 0.26 ppm MeOH, 0.076 ppm HCHO
(BLUE)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO    =           0.298,
NO2   =           0.089,
HCHO  =   0.0763,
MEOH  =   0.2649,
RCHO  =   0.0096,
PAR   =   0.2193,
ETH   =   0.1188,
OLE   =   0.0179,
TOL   =   0.0235,
XYL   =   0.0187,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =           0.0062,
CO    =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0984.LIX;
TEMPERATURE= (AUG 9 88)
    0:  296.2,    61:  296.7,   117:  299.3,   181:  303.6,
  237:  307.9,   301:  310.5,   357:  312.5,   365:  312.5,
  421:  313.1,   477:  313.5,   485:  313.3,   615:313.8;
WATER= (BLUE AUG 9 88)
    0: 29190.9,    57: 29988.7,   121: 32302.8,   177:
31071.3,
  185: 31530.6,   241: 31234.4,   297: 32065.3,   361:
32784.0,
  417: 33415.3,   481: 33273.7,   537: 32957.9,    615:
34061.0;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 9, 1984 1.30 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CALCHMW.PKS
CONC=
NO =    0.302,
NO2 =  0.087,
ALK4 = 0.0269,
ALK7 = 0.0213,
ETHE = 0.1726,
PRPE = 0.0266,
TBUT = 0.0073,
TOLU = 0.0366,
XYLE = 0.0214,
TMBZ = 0.0075,
HCHO = 0.0188,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =             0.0061,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0984.LIX;
TEMPERATURE= (AUG 9 88)
    0:  296.2,    61:  296.7,    117:  299.3,    181:  303.6,
  237:  307.9,   301:  310.5,    357:  312.5,    365:  312.5,
  421:  313.1,   477:  313.5,    485:  313.3,    615:313.8;
WATER= (RED AUG 9 88)
    0: 29342.4,    61: 30492.4,    117: 33238.5,    181:
32888.1,
  237: 33203.2,   245: 32853.4,    301: 33309.0,    357:
33664.7,
  421: 34463.3,   477: 34722.1,    485: 34206.8,    615:
34722.0;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 9, 1984  1.30 ppmC SYNAUTO (RED)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO =                   0.302,
NO2 =                  0.088,
PAR  =                 0.3200,
ETH   =                0.1726,
OLE    =               0.0266,
TOL     =              0.0366,
XYL      =             0.0288,
RCHO      =            0.0146,
HCHO       =           0.0188,
(background)
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0061,
CO    =        0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0984.LIX;
TEMPERATURE= (AUG 9 88)
    0:  296.2,    61:  296.7,    117:  299.3,    181:  303.6,
  237:  307.9,   301:  310.5,    357:  312.5,    365:  312.5,
  421:  313.1,   477:  313.5,    485:  313.3,    615:313.8;
WATER= (RED AUG 9 88)
    0: 29342.4,    61: 30492.4,   117: 33238.5,   181:
32888.1,
  237: 33203.2,   245: 32853.4,   301: 33309.0,   357:
33664.7,
  421: 34463.3,   477: 34722.1,   485: 34206.8,   615:
34722.0;
DILUTION=
0: 1.5E-4, 300: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
Aug 9, 1984 0.86 ppmC SYNAUTO, 0.26 ppm MeOH, 0.076 ppm HCHO
(BLUE)
C:\pkss\MECH\CalchmW.PKS
CONC=
NO     =          0.298,
NO2    =          0.089,
HCHO   =          0.0763,
MEOH   =          0.2619,
MEONO  =          0.003,
ALK4   =          0.0186,
ALK7   =          0.0145,
ETHE   =          0.1255,
PRPE   =          0.0179,
TBUT   =          0.0048,
TOLU   =          0.0235,
XYLE   =          0.0139,
TMBZ   =          0.0048,
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =          0.0062,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\AU0984.LIX;
TEMPERATURE= (AUG 9 88)
    0:  296.2,    61:  296.7,    117:  299.3,    181:  303.6,
  237:  307.9,   301:  310.5,    357:  312.5,    365:  312.5,
  421:  313.1,   477:  313.5,    485:  313.3,    615:313.8;
WATER= (BLUE AUG 9 88)
    0: 29190.9,    57: 29988.7,    121: 32302.8,    177:
31071.3,
  185: 31530.6,   241: 31234.4,    297: 32065.3,    361:
32784.0,
  417: 33415.3,   481: 33273.7,    537: 32957.9,    615:
34061.0;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 9, 1984 0.86 ppmC SYNAUTO, 0.26 ppm MeOH, 0.076 ppm HCHO
(BLUE)
C:\PKSS\MECH\CB42CHMW.PKS
CONC=
NO     =           0.298,
NO2    =           0.089,
HCHO   =   0.0763,
MEOH   =   0.2619,
MEONO  =   0.003,
RCHO   =   0.0096,
PAR    =   0.2193,
ETH    =   0.1188,
OLE    =   0.0179,
TOL    =   0:0235,
XYL    =   0.0187,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =           0.0062,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\AU0984.LIX;
TEMPERATURE= (AUG 9 88)
    0:  296.2,    61:  296.7,    117:  299.3,    181:  303.6,
  237:  307.9,   301:  310.5,    357:  312.5,    365:  312.5,
  421:  313.1,   477:  313.5,    485:  313.3,    615:313.8;
WATER= (BLUE AUG 9 88)
    0: 29190.9,    57: 29988.7,   121: 32302.8,   177:
31071.3,
  185: 31530.6,   241: 31234.4,   297: 32065.3,   361:
32784.0,
  417: 33415.3,   481: 33273.7,   537: 32957.9,    615:
34061.0;
DILUTION=
  0: 1.5E-4,610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
August 22, 1984 3.2 ppmC SYNURBAN (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =        0.254,
NO2     =        0.070,
ETHE    =        0.1104 ,
PRPE    =        0.0557 ,
TBUT    =        0.0202 ,
ALK4    =        0.1166 ,
ALK7    =        0.1973 ,
TOLU    =        0.0576 ,
XYLE    =        0.0364 ,
TMBZ    =        0.0149 ,
HCHO    =        0.0556 ,
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =             0.0049,
CO      =             0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,    122:  294.3,    330:  307.0,
  362:  308.2,   418:  308.6,    482:  308.4,    538:  308.3,
612:  306.6;
WATER= (RED AUG 22 84)
    0: 7824.0,    58: 7717.2,     66: 7747.6,    114: 7901.0,
122: 7839.4,
  354: 8336.5,   362: 8500.0,    418: 8844.0,    426: 8903.9,
  474: 9235.7,   482: 9369.7,    538: 9773.1,    546: 9819.9,
612: 10231.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 22, 1984 3.2 ppmC SYNURBAN (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =            0.254,
NO2    =           0.070,
ETH      =         0.1104 ,
OLE      =         0.0557 ,
PAR      =         1.8811 ,
TOL      =         0.0576 ,
XYL      =         0.0513 ,
HCHO     =         0.0556 ,
RCHO     =         0.0318 ,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0049,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,   122:  294.3,   330:  307.0,
  362:  308.2,   418:  308.6,   482:  308.4,   538:  308.3,
612:  306.6;
WATER= (RED AUG 22 84)
    0: 7824.0,    58: 7717.2,    66: 7747.6,   114: 7901.0,
122: 7839.4,
  354: 8336.5,   362: 8500.0,   418: 8844.0,   426: 8903.9,
  474: 9235.7,   482: 9369.7,   538: 9773.1,   546: 9819.9,
612: 10231.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 22, 1984 2.1 ppmC SYNURBAN, 0.87 PPM MEOH, 0.13 PPM
HCHO (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO       =         0.254,
NO2      =         0.070,
ETHE     =         0.0704,
PRPE     =         0.0344,
TBUT     =         0.0151,
ALK4     =         0.0769,
ALK7     =         0.1302,
TOLU     =         0.0396,
XYLE     =         0.0262,
TMBZ     =         0.0095,
HCHO     =         0.1301,
MEOH     =         0.8761,
      (Surface NMHC = 0.0380 ppmC)
ALK4     =   0.0201,
ETHE     =   0.0009,
PRPE     =   0.0006,
TOLU     =   0.0004,
XYLE     =   0.0003,
HCHO     =   0.0038,
ALD2     =   0.0030,
HONO     =           0.0049,
CO       =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,    122:  294.3,    330:  307.0,
  362:  308.2,   418:  308.6,    482:  308.4,    538:  308.3,
612:  306.6;
WATER= (BLUE AUG 22 84)
    0: 10853.0,    54: 10935.9,    62: 10863.4,   118:
10915.1,  126: 10801.6,
  358: 11488.9,   366: 11543.5,   414: 11764.3,   422:
11797.8,
  478: 12276.5,   486: 12334.8,   534: 12750.3,   542:
12908.2,  616: 13317.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=            600;
FINISH
!
```

```
Aug 22, 1984 2.1 ppmC SYNURBAN, 0.87 PPM MEOH, 0.13 HCHO
(BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO   =           0.254,
NO2    =         0.070,
ETH      =       0.0704,
OLE      =       0.0344,
PAR      =       1.2377,
TOL      =       0.0396,
XYL      =       0.0357,
HCHO     =       0.1301,
MEOH     =       0.8761,
RCHO     =       0.0237,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0049,
CO     =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,   122:  294.3,   330:  307.0,
  362:  308.2,   418:  308.6,   482:  308.4,   538:  308.3,
612:  306.6;
WATER= (BLUE AUG 22 84)
    0: 10853.0,    54: 10935.9,    62: 10863.4,   118:
10915.1,  126: 10801.6,
  358: 11488.9,   366: 11543.5,   414: 11764.3,   422:
11797.8,
  478: 12276.5,   486: 12334.8,   534: 12750.3,   542:
12908.2,  616: 13317.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 22, 1984 3.2 ppmC SYNURBAN (RED)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO     =        0.254,
NO2    =        0.070,
ETH    =        0.1104 ,
OLE    =        0.0759 ,
ALK    =        0.3139 ,
AROM   =        0.1221 ,
HCHO   =        0.0556 ,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0049,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,   122:  294.3,   330:  307.0,
  362:  308.2,   418:  308.6,   482:  308.4,   538:  308.3,
612:  306.6;
EMISSIONS=2#
  0: 3.47E-3, 1.20E-5,
 58: 3.46E-3, 1.20E-5,
122: 3.40E-3, 1.15E-5,
330: 3.26E-3, 1.06E-5,
362: 3.24E-3, 1.05E-5,
538: 3.24E-3, 1.05E-5,
612: 3.26E-3, 1.06E-5;
WATER= (RED AUG 22 84)
    0: 7824.0,    58: 7717.2,    66: 7747.6,   114: 7901.0,
122: 7839.4,
  354: 8336.5,   362: 8500.0,   418: 8844.0,   426: 8903.9,
  474: 9235.7,   482: 9369.7,   538: 9773.1,   546: 9819.9,
612: 10231.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 22, 1984 3.2 ppmC SYNURBAN (RED)
C:\PKSS\mech\CITCHMW2.pks
CONC:
NO      =        0.254,
NO2     =        0.070,
ETH     =        0.1104 ,
OLE     =        0.0759 ,
ALK     =        0.3139 ,
AROM    =        0.1221 ,
HCHO    =        0.0556 ,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0049,
CO      =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,   122:  294.3,   330:  307.0,
  362:  308.2,   418:  308.6,   482:  308.4,   538:  308.3,
612:  306.6;
EMISSIONS=2#
  0: 3.47E-3, 1.20E-5,
 58: 3.46E-3, 1.20E-5,
122: 3.40E-3, 1.15E-5,
330: 3.26E-3, 1.06E-5,
362: 3.24E-3, 1.05E-5,
538: 3.24E-3, 1.05E-5,
612: 3.26E-3, 1.06E-5;
WATER= (RED AUG 22 84)
    0: 7824.0,    58: 7717.2,    66: 7747.6,   114: 7901.0,
122: 7839.4,
  354: 8336.5,   362: 8500.0,   418: 8844.0,   426: 8903.9,
  474: 9235.7,   482: 9369.7,   538: 9773.1,   546: 9819.9,
612: 10231.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 22, 1984 2.1 ppmC SYNURBAN, 0.87 PPM MEOH, 0.13 PPM
HCHO (BLUE)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO      =        0.254,
NO2     =        0.070,
ETH     =        0.0704,
OLE     =        0.0495,
ALK     =        0.2071,
AROM    =        0.0844,
HCHO    =        0.1301,
MEOH    =        0.8761,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO    =          0.0049,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2284.1Ix;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,   122:  294.3,   330:  307.0,
  362:  308.2,   418:  308.6,   482:  308.4,   538:  308.3,
612:  306.6;
EMISSIONS=2#
  0: 3.47E-3, 1.20E-5,
 58: 3.46E-3, 1.20E-5,
122: 3.40E-3, 1.15E-5,
330: 3.26E-3, 1.06E-5,
362: 3.24E-3, 1.05E-5,
538: 3.24E-3, 1.05E-5,
612: 3.26E-3, 1.06E-5;
WATER= (BLUE AUG 22 84)
    0: 10853.0,    54: 10935.9,    62: 10863.4,    118:
10915.1,  126: 10801.6,
  358: 11488.9,   366: 11543.5,   414: 11764.3,   422:
11797.8,
  478: 12276.5,   486: 12334.8,   534: 12750.3,   542:
12908.2,  616: 13317.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 22, 1984 2.1 ppmC SYNURBAN, 0.87 PPM MEOH, 0.13 PPM
HCHO (BLUE)
C:\PKSS\mech\CITCHMW2.pks
CONC:
NO      =         0.254,
NO2     =         0.070,
ETH     =         0.0704,
OLE     =         0.0495,
ALK     =         0.2071,
AROM    =         0.0844,
HCHO    =         0.1301,
MEOH    =         0.8761,
        (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO    =          0.0049,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,   122:  294.3,   330:  307.0,
  362:  308.2,   418:  308.6,   482:  308.4,   538:  308.3,
612:  306.6;
EMISSIONS=2#
  0: 3.47E-3, 1.20E-5,
 58: 3.46E-3, 1.20E-5,
122: 3.40E-3, 1.15E-5,
330: 3.26E-3, 1.06E-5,
362: 3.24E-3, 1.05E-5,
538: 3.24E-3, 1.05E-5,
612: 3.26E-3, 1.06E-5;
WATER= (BLUE AUG 22 84)
    0: 10853.0,    54: 10935.9,    62: 10863.4,   118:
10915.1,  126: 10801.6,
  358: 11488.9,   366: 11543.5,   414: 11764.3,   422:
11797.8,
  478: 12276.5,   486: 12334.8,   534: 12750.3,   542:
12908.2,  616: 13317.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 22, 1984 3.2 ppmC SYNURBAN (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =        0.254,
NO2     =        0.070,
ETHE    =        0.1104 ,
PRPE    =        0.0557 ,
TBUT    =        0.0202 ,
ALK4    =        0.1166 ,
ALK7    =        0.1973 ,
TOLU    =        0.0576 ,
XYLE    =        0.0364 ,
TMBZ    =        0.0149 ,
HCHO    =        0.0556 ,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0049,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,   122:  294.3,   330:  307.0,
  362:  308.2,   418:  308.6,   482:  308.4,   538:  308.3,
612:  306.6;
WATER= (RED AUG 22 84)
    0: 7824.0,    58: 7717.2,    66: 7747.6,   114: 7901.0,
122: 7839.4,
  354: 8336.5,   362: 8500.0,   418: 8844.0,   426: 8903.9,
  474: 9235.7,   482: 9369.7,   538: 9773.1,   546: 9819.9,
612: 10231.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 22, 1984 3.2 ppmC SYNURBAN (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =            0.254,
NO2    =           0.070,
ETH      =         0.1104 ,
OLE      =         0.0557 ,
PAR      =         1.8811 ,
TOL      =         0.0576 ,
XYL      =         0.0513 ,
HCHO     =         0.0556 ,
RCHO     =         0.0318 ,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0049,
CO     =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,     58:  289.1,    122:  294.3,    330:  307.0,
  362:  308.2,   418:  308.6,    482:  308.4,    538:  308.3,
612:  306.6;
WATER= (RED AUG 22 84)
    0: 7824.0,     58: 7717.2,     66: 7747.6,    114: 7901.0,
122: 7839.4,
  354: 8336.5,   362: 8500.0,    418: 8844.0,    426: 8903.9,
  474: 9235.7,   482: 9369.7,    538: 9773.1,    546: 9819.9,
612: 10231.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
August 22, 1984 2.1 ppmC SYNURBAN, 0.87 PPM MEOH, 0.13 PPM
HCHO (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =          0.254,
NO2     =          0.070,
ETHE    =          0.0704,
PRPE    =          0.0344,
TBUT    =          0.0151,
ALK4    =          0.0769,
ALK7    =          0.1302,
TOLU    =          0.0396,
XYLE    =          0.0262,
TMBZ    =          0.0095,
HCHO    =          0.1301,
MEOH    =          0.8661,
MEONO   =          0.010,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =    0.0201,
ETHE    =    0.0009,
PRPE    =    0.0006,
TOLU    =    0.0004,
XYLE    =    0.0003,
HCHO    =    0.0038,
ALD2    =    0.0030,
HONO    =            0.0049,
CO      =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,   122:  294.3,   330:  307.0,
  362:  308.2,   418:  308.6,   482:  308.4,   538:  308.3,
612:  306.6;
WATER= (BLUE AUG 22 84)
    0: 10853.0,    54: 10935.9,    62: 10863.4,   118:
10915.1,  126: 10801.6,
  358: 11488.9,   366: 11543.5,   414: 11764.3,   422:
11797.8,
  478: 12276.5,   486: 12334.8,   534: 12750.3,   542:
12908.2,  616: 13317.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 22, 1984 2.1 ppmC SYNURBAN, 0.87 PPM MEOH, 0.13 HCHO
(BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =            0.254,
NO2    =           0.070,
ETH      =         0.0704,
OLE      =         0.0344,
PAR      =         1.2377,
TOL      =         0.0396,
XYL      =         0.0357,
HCHO     =         0.1301,
MEOH     =         0.8661,
MEONO    =         0.010,
RCHO     =         0.0237,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0049,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL.HCHO.RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2284.lIx;
TEMPERATURE= (AUG 22 84)
    0:  288.4,    58:  289.1,   122:  294.3,   330:  307.0,
  362:  308.2,   418:  308.6,   482:  308.4,   538:  308.3,
612:  306.6;
WATER= (BLUE AUG 22 84)
    0: 10853.0,    54: 10935.9,    62: 10863.4,   118:
10915.1,  126: 10801.6,
  358: 11488.9,   366: 11543.5,   414: 11764.3,   422:
11797.8,
  478: 12276.5,   486: 12334.8,   534: 12750.3,   542:
12908.2,  616: 13317.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
August 25, 1984 1/3 MEOH W/10% HCHO (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =        0.269,
NO2     =        0.076,
ALK4    =        0.017,
ALK7    =        0.051,
ETHE    =        0.039,
PRPE    =        0.017,
TBUT    =        0.006,
TOLU    =        0.015,
XYLE    =        0.010,
TMBZ    =        0.003,
HCHO    =        0.043,
MEOH    =        0.295,
(NROG   =        0.003,
 MISS   =        -.004)
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0053,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,   120:  292.7,   180:  295.4,
  240:  301.8,   300:  304.6,   360:  304.9,   420:  305.9,
  480:  306.0,   540:  305.3,   600:  303.9;
WATER= (RED AUG 25 84)
    7: 19118.5,   23: 22469.5,   71: 22896.4,  135: 23170.9,
  191: 23240.1,  263: 23379.1,  351: 23402.5,  415: 23449.1,
  519: 23802.4,  599: 23802.4;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
Aug 25, 1984 1/3 MEOH W/10% HCHO (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =           0.269,
NO2    =          0.076,
PAR      =        0.443,
ETH      =        0.039,
OLE      =        0.018,
TOL      =        0.015,
XYL      =        0.013,
HCHO     =        0.043,
RCHO     =        0.009,
MEOH     =        0.295,
(NR      =        0.021,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0053,
CO     =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH.OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,    120:  292.7,    180:  295.4,
  240:  301.8,   300:  304.6,    360:  304.9,    420:  305.9,
  480:  306.0,   540:  305.3,    600:  303.9;
WATER= (RED AUG 25 84)
    7: 19118.5,    23: 22469.5,    71: 22896.4,   135: 23170.9,
  191: 23240.1,   263: 23379.1,   351: 23402.5,   415: 23449.1,
  519: 23802.4,   599: 23802.4;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 25, 1984 1.09 PPMC SYNURBAN (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO     =        0.262,
NO2    =        0.070,
ETHE   =        0.058,
PRPE   =        0.024,
TBUT   =        0.009,
ALK4   =        0.026,
ALK7   =        0.068,
TOLU   =        0.020,
XYLE   =        0.012,
TMBZ   =        0.005,
HCHO   =        0.019,
(NROG  =        0.004,
 MISS  =        -.001)
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =           0.0049,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,    120:  292.7,    180:  295.4,
  240:  301.8,   300:  304.6,    360:  304.9,    420:  305.9,
  480:  306.0,   540:  305.3,    600:  303.9;
WATER= (BLUE AUG 25 84)
    0: 19645.3,   10: 18897.5,    20: 22248.4,    75: 22336.6,
  195: 22469.5,  211: 22581.0,   323: 22760.7,   411: 22942.0,
  499: 23147.9,  600: 23193.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 25, 1984 1.09 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =          0.262,
NO2    =         0.070,
ETH      =       0.058,
OLE      =       0.024,
PAR      =       0.606,
TOL      =       0.020,
XYL      =       0.017,
HCHO     =       0.019,
RCHO     =       0.014,
(NR       =       0.025,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0049,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,   120:  292.7,   180:  295.4,
  240:  301.8,   300:  304.6,   360:  304.9,   420:  305.9,
  480:  306.0,   540:  305.3,   600:  303.9;
WATER= (BLUE AUG 25 84)
    0: 19645.3,   10: 18897.5,   20: 22248.4,   75: 22336.6,
  195: 22469.5,  211: 22581.0,  323: 22760.7,  411: 22942.0,
  499: 23147.9,  600: 23193.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 25, 1984 1/3 MEOH W/10% HCHO (RED)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO      =         0.269,
NO2     =         0.076,
ALK    =         0.068,
ETH    =         0.039,
OLE    =         0.024,
AROM   =         0.0316,
HCHO    =         0.043,
MEOH    =         0.295,
       (Surface NMHC = 0.0380 ppmC)
ALK    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
AROM   =   0.0007,
HCHO    =   0.0038,
RCHO    =   0.0030,
HONO    =             0.0053,
CO      =             0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,   120:  292.7,   180:  295.4,
  240:  301.8,   300:  304.6,   360:  304.9,   420:  305.9,
  480:  306.0,   540:  305.3,   600:  303.9;
EMISSIONS=2#
  0: 3.42E-3, 1.17E-5,
 30: 3.42E-3, 1.17E-5,
120: 3.42E-3, 1.17E-5,
180: 3.38E-3, 1.14E-5,
240: 3.31E-3, 1.10E-5,
300: 3.28E-3, 1.08E-5,
360: 3.28E-3, 1.08E-5,
420: 3.27E-3, 1.07E-5,
480: 3.27E-3, 1.07E-5,
540: 3.28E-3, 1.07E-5,
600: 3.29E-3, 1.08E-5;
WATER= (RED AUG 25 84)
    7: 19118.5,   23: 22469.5,   71: 22896.4,  135: 23170.9,
  191: 23240.1,  263: 23379.1,  351: 23402.5,  415: 23449.1,
  519: 23802.4,  599: 23802.4;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 25, 1984 1/3 MEOH W/10% HCHO (RED)
C:\PKSS\mech\citchmw2.pks
CONC:
NO      =        0.269,
NO2     =        0.076,
ALK    =        0.068,
ETH    =        0.039,
OLE    =        0.024,
AROM   =        0.0316,
HCHO    =        0.043,
MEOH    =        0.295,
      (Surface NMHC = 0.0380 ppmC)
ALK    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
AROM   =   0.0007,
HCHO    =   0.0038,
RCHO    =   0.0030,
HONO    =          0.0053,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,    120:  292.7,    180:  295.4,
  240:  301.8,   300:  304.6,    360:  304.9,    420:  305.9,
  480:  306.0,   540:  305.3,    600:  303.9;
EMISSIONS=2#
  0: 3.42E-3, 1.17E-5,
 30: 3.42E-3, 1.17E-5,
120: 3.42E-3, 1.17E-5,
180: 3.38E-3, 1.14E-5,
240: 3.31E-3, 1.10E-5,
300: 3.28E-3, 1.08E-5,
360: 3.28E-3, 1.08E-5,
420: 3.27E-3, 1.07E-5,
480: 3.27E-3, 1.07E-5,
540: 3.28E-3, 1.07E-5,
600: 3.29E-3, 1.08E-5;
WATER= (RED AUG 25 84)
    7: 19118.5,   23: 22469.5,   71: 22896.4,   135: 23170.9,
  191: 23240.1,  263: 23379.1,  351: 23402.5,   415: 23449.1,
  519: 23802.4,  599: 23802.4;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 25, 1984 1.09 PPMC SYNURBAN (BLUE)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO     =         0.262,
NO2    =         0.070,
ETH    =         0.058,
OLE    =         0.033,
ALK    =         0.092,
AROM   =         0.0423,
HCHO   =         0.019,
        (Surface NMHC = 0.0380 ppmC)
ALK    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
AROM   =   0.0007,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO    =           0.0049,
CO      =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,     30:  292.3,    120:  292.7,    180:  295.4,
  240:  301.8,    300:  304.6,    360:  304.9,    420:  305.9,
  480:  306.0,    540:  305.3,    600:  303.9;
EMISSIONS=2#
  0: 3.42E-3, 1.17E-5,
 30: 3.42E-3, 1.17E-5,
120: 3.42E-3, 1.17E-5,
180: 3.38E-3, 1.14E-5,
240: 3.31E-3, 1.10E-5,
300: 3.28E-3, 1.08E-5,
360: 3.28E-3, 1.08E-5,
420: 3.27E-3, 1.07E-5,
480: 3.27E-3, 1.07E-5,
540: 3.28E-3, 1.07E-5,
600: 3.29E-3, 1.08E-5;
WATER= (BLUE AUG 25 84)
    0: 19645.3,   10: 18897.5,   20: 22248.4,   75: 22336.6,
  195: 22469.5,  211: 22581.0,  323: 22760.7,  411: 22942.0,
  499: 23147.9,  600: 23193.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
August 25, 1984 1.09 PPMC SYNURBAN (BLUE)
C:\PKSS\mech\citchmw2.pks
CONC:
NO     =        0.262,
NO2    =        0.070,
ETH    =        0.058,
OLE    =        0.033,
ALK    =        0.092,
AROM   =        0.0423,
HCHO   =        0.019,
        (Surface NMHC = 0.0380 ppmC)
ALK    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
AROM   =   0.0007,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO    =           0.0049,
CO      =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,   120:  292.7,   180:  295.4,
  240:  301.8,   300:  304.6,   360:  304.9,   420:  305.9,
  480:  306.0,   540:  305.3,   600:  303.9;
EMISSIONS=2#
  0: 3.42E-3, 1.17E-5,
 30: 3.42E-3, 1.17E-5,
120: 3.42E-3, 1.17E-5,
180: 3.38E-3, 1.14E-5,
240: 3.31E-3, 1.10E-5,
300: 3.28E-3, 1.08E-5,
360: 3.28E-3, 1.08E-5,
420: 3.27E-3, 1.07E-5,
480: 3.27E-3, 1.07E-5,
540: 3.28E-3, 1.07E-5,
600: 3.29E-3, 1.08E-5;
WATER= (BLUE AUG 25 84)
    0: 19645.3,   10: 18897.5,   20: 22248.4,   75: 22336.6,
  195: 22469.5,  211: 22581.0,  323: 22760.7,  411: 22942.0,
  499: 23147.9,  600: 23193.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 25, 1984 1/3 MEOH W/10% HCHO (RED)
C:\PKSS\MECH\CALCHMK.PKS
CONC:
NO      =        0.269,
NO2     =        0.076,
ALK4    =        0.017,
ALK7    =        0.051,
ETHE    =        0.039,
PRPE    =        0.017,
TBUT    =        0.006,
TOLU    =        0.015,
XYLE    =        0.010,
TMBZ    =        0.003,
HCHO    =        0.043,
MEOH    =        0.295,
(NROG   =        0.003,
 MISS   =        -.004)
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0053,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,   120:  292.7,   180:  295.4,
  240:  301.8,   300:  304.6,   360:  304.9,   420:  305.9,
  480:  306.0,   540:  305.3,   600:  303.9;
WATER= (RED AUG 25 84)
    7: 19118.5,   23: 22469.5,   71: 22896.4,  135: 23170.9,
  191: 23240.1,  263: 23379.1,  351: 23402.5,  415: 23449.1,
  519: 23802.4,  599: 23802.4;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 25, 1984 1/3 MEOH W/10% HCHO (RED)
C:\PKSS\MECH\CB42CHMK.PKS
CONC:
NO    =           0.269,
NO2    =          0.076,
PAR      =        0.443,
ETH      =        0.039,
OLE      =        0.018,
TOL      =        0.015,
XYL      =        0.013,
HCHO     =        0.043,
RCHO     =        0.009,
MEOH     =        0.295,
(NR      =        0.021,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0053,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,   120:  292.7,   180:  295.4,
  240:  301.8,   300:  304.6,   360:  304.9,   420:  305.9,
  480:  306.0,   540:  305.3,   600:  303.9;
WATER= (RED AUG 25 84)
    7: 19118.5,   23: 22469.5,   71: 22896.4,  135: 23170.9,
  191: 23240.1,  263: 23379.1,  351: 23402.5,  415: 23449.1,
  519: 23802.4,  599: 23802.4;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 25, 1984 1.09 PPMC SYNURBAN (BLUE)
C:\PKSS\MECH\CALCHMK.PKS
CONC:
NO      =        0.262,
NO2     =        0.070,
ETHE    =        0.058,
PRPE    =        0.024,
TBUT    =        0.009,
ALK4    =        0.026,
ALK7    =        0.068,
TOLU    =        0.020,
XYLE    =        0.012,
TMBZ    =        0.005,
HCHO    =        0.019,
(NROG   =        0.004,
 MISS   =        -.001)
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0049,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\au2584.1Ix;
TEMPERATURE= (AUG 25 84)
    0:  292.2,     30:  292.3,    120:  292.7,    180:  295.4,
  240:  301.8,    300:  304.6,    360:  304.9,    420:  305.9,
  480:  306.0,    540:  305.3,    600:  303.9;
WATER= (BLUE AUG 25 84)
    0: 19645.3,    10: 18897.5,    20: 22248.4,    75: 22336.6,
  195: 22469.5,   211: 22581.0,   323: 22760.7,   411: 22942.0,
  499: 23147.9,   600: 23193.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 25, 1984 1.09 ppmC SYNURBAN (BLUE)
C:\PKSS\MECH\CB42CHMK.PKS
CONC:
NO    =           0.262,
NO2    =          0.070,
ETH      =        0.058,
OLE      =        0.024,
PAR      =        0.606,
TOL      =        0.020,
XYL      =        0.017,
HCHO     =        0.019,
RCHO     =        0.014,
(NR       =        0.025,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0049,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,   120:  292.7,   180:  295.4,
  240:  301.8,   300:  304.6,   360:  304.9,   420:  305.9,
  480:  306.0,   540:  305.3,   600:  303.9;
WATER= (BLUE AUG 25 84)
    0: 19645.3,   10: 18897.5,   20: 22248.4,   75: 22336.6,
  195: 22469.5,  211: 22581.0,  323: 22760.7,  411: 22942.0,
  499: 23147.9,  600: 23193.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
August 25, 1984 1/3 MEOH W/10% HCHO (RED)
C:\PKSS\MECH\CALCHMN.PKS
CONC:
NO     =         0.269,
NO2    =         0.076,
ALK4   =         0.017,
ALK7   =         0.051,
ETHE   =         0.039,
PRPE   =         0.017,
TBUT   =         0.006,
TOLU   =         0.015,
XYLE   =         0.010,
TMBZ   =         0.003,
HCHO   =         0.043,
MEOH   =         0.295,
(NROG  =         0.003,
 MISS  =         -.004)
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =          0.0053,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,    120:  292.7,    180:  295.4,
  240:  301.8,   300:  304.6,    360:  304.9,    420:  305.9,
  480:  306.0,   540:  305.3,    600:  303.9;
WATER= (RED AUG 25 84)
    7: 19118.5,   23: 22469.5,    71: 22896.4,   135: 23170.9,
  191: 23240.1,  263: 23379.1,   351: 23402.5,   415: 23449.1,
  519: 23802.4,  599: 23802.4;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 25, 1984 1/3 MEOH W/10% HCHO (RED)
C:\PKSS\MECH\CB42CHMN.PKS
CONC:
NO   =           0.269,
NO2   =          0.076,
PAR     =        0.443,
ETH     =        0.039,
OLE     =        0.018,
TOL     =        0.015,
XYL     =        0.013,
HCHO    =        0.043,
RCHO    =        0.009,
MEOH    =        0.295,
(NR     =        0.021,)
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0053,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,   120:  292.7,   180:  295.4,
  240:  301.8,   300:  304.6,   360:  304.9,   420:  305.9,
  480:  306.0,   540:  305.3,   600:  303.9;
WATER= (RED AUG 25 84)
    7: 19118.5,   23: 22469.5,   71: 22896.4,  135: 23170.9,
  191: 23240.1,  263: 23379.1,  351: 23402.5,  415: 23449.1,
  519: 23802.4,  599: 23802.4;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
Aug 25, 1984 1.09 ppmC SYNURBAN (BLUE)
C:\PKSS\MECH\CB42CHMN.PKS
CONC:
NO    =           0.262,
NO2    =          0.070,
ETH      =        0.058,
OLE      =        0.024,
PAR      =        0.606,
TOL      =        0.020,
XYL      =        0.017,
HCHO     =        0.019,
RCHO     =        0.014,
(NR       =        0.025,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0049,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\au2584.lIx;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,   120:  292.7,   180:  295.4,
  240:  301.8,   300:  304.6,   360:  304.9,   420:  305.9,
  480:  306.0,   540:  305.3,   600:  303.9;
WATER= (BLUE AUG 25 84)
    0: 19645.3,   10: 18897.5,    20: 22248.4,    75: 22336.6,
  195: 22469.5,  211: 22581.0,   323: 22760.7,   411: 22942.0,
  499: 23147.9,  600: 23193.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
August 25, 1984 1.09 PPMC SYNURBAN (BLUE)
C:\PKSS\MECH\CALCHMN.PKS
CONC:
NO      =         0.262,
NO2     =         0.070,
ETHE    =         0.058,
PRPE    =         0.024.
TBUT    =         0.009,
ALK4    =         0.026,
ALK7    =         0.068,
TOLU    =         0.020,
XYLE    =         0.012,
TMBZ    =         0.005,
HCHO    =         0.019,
(NROG   =         0.004,
 MISS   =         -.001)
      (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0049,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4.ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\au2584.1Ix;
TEMPERATURE= (AUG 25 84)
    0:  292.2,    30:  292.3,   120:  292.7,   180:  295.4,
  240:  301.8,   300:  304.6,   360:  304.9,   420:  305.9,
  480:  306.0,   540:  305.3,   600:  303.9;
WATER= (BLUE AUG 25 84)
    0: 19645.3,   10: 18897.5,   20: 22248.4,   75: 22336.6,
  195: 22469.5,  211: 22581.0,  323: 22760.7,  411: 22942.0,
  499: 23147.9,  600: 23193.9;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=        600;
FINISH
!
```

```
September 1, 1984 2.68 ppmC SYNURBAN, 0.97 ppmC MeOH (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =   0.252,
NO2     =   0.062,
ETHE    =   0.0804,
PRPE    =   0.0358,
TBUT    =   0.0132,
ALK4    =   0.2034,
ALK7    =   0.1377,
TOLU    =   0.0392,
XYLE    =   0.0256,
TMBZ    =   0.0086,
HCHO    =   0.037,
MEOH    =   0.9660,
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0043,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0184.lix;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,   123:  293.8,   179:  299.1,
  235:  302.8,   243:  303.1,   299:  305.4,   363:  307.1,
  419:  307.8,   483:  307.2,   539:  307.4,   613:  306.8;
WATER = (RED SEP 1 84)
    0: 8582.8,    59: 8716.7,   123: 8835.4,   179: 8946.9,
  243: 9007.5,   299: 9414.8,   355: 9333.8,   363: 9505.5,
  419: 9857.5,   483: 10038.0,  539: 10143.9,  613: 10448.0;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=        600;
FINISH
!
```

```
September 1, 1984 2.68 ppmC SYNURBAN, 0.97 ppmC MeOH (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =   0.252,
NO2   =   0.062,
ETH   =   0.0804,
OLE   =   0.0358,
PAR   =   1.7838,
TOL   =   0.0392,
XYL   =   0.0341,
HCHO  =   0.0370,
MEOH  =   0.9660,
RCHO  =   0.0202,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0043,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0184.LIX;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,   123:  293.8,   179:  299.1,
  235:  302.8,   243:  303.1,   299:  305.4,   363:  307.1,
  419:  307.8,   483:  307.2,   539:  307.4,   613:  306.8;
WATER = (RED SEP 1 84)
    0: 8582.8,    59: 8716.7,   123: 8835.4,   179: 8946.9,
  243: 9007.5,   299: 9414.8,   355: 9333.8,   363: 9505.5,
  419: 9857.5,   483: 10038.0,  539: 10143.9,  613: 10448.0;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 1, 1984 3.26 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO    =              0.243,
NO2    =             0.059,
ETHE     =        0.1080,
PRPE     =        0.0509,
TBUT     =        0.0192,
ALK4     =        0.1427,
ALK7     =        0.1954,
TOLU     =        0.0590,
XYLE     =        0.0373,
TMBZ     =        0.0122,
HCHO     =        0.0550,
        (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0041,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0184.LIX;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,    123:  293.8,    179:  299.1,
  235:  302.8,   243:  303.1,    299:  305.4,    363:  307.1,
  419:  307.8,   483:  307.2,    539:  307.4,    613:  306.8;
WATER= (BLUE SEP 1 84)
    0: 14110.4,    63: 14380.7,   119: 15695.5,   183:
15487.6,
  239: 15785.6,   295: 15921.7,   303: 15770.6,   359:
16043.7,
  423: 16228.7,   479: 16510.3,   543: 16845.7,   615:
17221.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 1, 1984 3.26 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =   0.243,
NO2   =   0.059,
ETH   =   0.1080,
OLE   =   0.0509,
PAR   =   1.9587,
TOL   =   0.0590,
XYL   =   0.0495,
HCHO  =   0.0550,
RCHO  =   0.0299,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0041,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0184.lix;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,   123:  293.8,   179:  299.1,
  235:  302.8,   243:  303.1,   299:  305.4,   363:  307.1,
  419:  307.8,   483:  307.2,   539:  307.4,   613:  306.8;
WATER= (BLUE SEP 1 84)
    0: 14110.4,    63: 14380.7,   119: 15695.5,   183:
15487.6,
  239: 15785.6,   295: 15921.7,   303: 15770.6,   359:
16043.7,
  423: 16228.7,   479: 16510.3,   543: 16845.7,   615:
17221.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 1, 1984 2.68 ppmC SYNURBAN, 0.97 ppmC MeOH (RED)
C:\PKSS\MECH\CALCHMK.PKS
CONC:
NO      =   0.252,
NO2     =   0.062,
ETHE    =   0.0804,
PRPE    =   0.0358,
TBUT    =   0.0132,
ALK4    =   0.2034,
ALK7    =   0.1377,
TOLU    =   0.0392,
XYLE    =   0.0256,
TMBZ    =   0.0086,
HCHO    =   0.037,
MEOH    =   0.9660,
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =            0.0043,
CO     =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0184.lix;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,    123:  293.8,    179:  299.1,
  235:  302.8,   243:  303.1,    299:  305.4,    363:  307.1,
  419:  307.8,   483:  307.2,    539:  307.4,    613:  306.8;
WATER = (RED SEP 1 84)
    0: 8582.8,    59: 8716.7,    123: 8835.4,    179: 8946.9,
  243: 9007.5,   299: 9414.8,    355: 9333.8,    363: 9505.5,
  419: 9857.5,   483: 10038.0,   539: 10143.9,   613: 10448.0;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 1, 1984 2.68 ppmC SYNURBAN, 0.97 ppmC MeOH (RED)
C:\PKSS\MECH\CB42CHMK.PKS
CONC:
NO    =   0.252,
NO2   =   0.062,
ETH   =   0.0804,
OLE   =   0.0358,
PAR   =   1.7838,
TOL   =   0.0392,
XYL   =   0.0341,
HCHO  =   0.0370,
MEOH  =   0.9660,
RCHO  =   0.0202,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0043,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0184.LIX;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,   123:  293.8,   179:  299.1,
  235:  302.8,   243:  303.1,   299:  305.4,   363:  307.1,
  419:  307.8,   483:  307.2,   539:  307.4,   613:  306.8;
WATER = (RED SEP 1 84)
    0: 8582.8,    59: 8716.7,   123: 8835.4,   179: 8946.9,
  243: 9007.5,   299: 9414.8,   355: 9333.8,   363: 9505.5,
  419: 9857.5,   483: 10038.0,  539: 10143.9,  613: 10448.0;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 1, 1984 3.26 ppmC SYNURBAN (BLUE)
C:\PKSS\MECH\CALCHMK.PKS
CONC:
NO    =                0.243,
NO2    =               0.059,
ETHE     =         0.1080,
PRPE     =         0.0509,
TBUT     =         0.0192,
ALK4     =         0.1427,
ALK7     =         0.1954,
TOLU     =         0.0590,
XYLE     =         0.0373,
TMBZ     =         0.0122,
HCHO     =         0.0550,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =              0.0041,
CO    =              0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0184.LIX;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,    123:  293.8,    179:  299.1,
  235:  302.8,   243:  303.1,    299:  305.4,    363:  307.1,
  419:  307.8,   483:  307.2,    539:  307.4,    613:  306.8;
WATER= (BLUE SEP 1 84)
    0: 14110.4,     63: 14380.7,    119: 15695.5,    183:
15487.6,
  239: 15785.6,    295: 15921.7,    303: 15770.6,    359:
16043.7,
  423: 16228.7,    479: 16510.3,    543: 16845.7,    615:
17221.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 1, 1984 3.26 ppmC SYNURBAN (BLUE)
C:\PKSS\MECH\CB42CHMK.PKS
CONC:
NO    =   0.243,
NO2   =   0.059,
ETH   =   0.1080,
OLE   =   0.0509,
PAR   =   1.9587,
TOL   =   0.0590,
XYL   =   0.0495,
HCHO  =   0.0550,
RCHO  =   0.0299,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0041,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0184.lix;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,   123:  293.8,   179:  299.1,
  235:  302.8,   243:  303.1,   299:  305.4,   363:  307.1,
  419:  307.8,   483:  307.2,   539:  307.4,   613:  306.8;
WATER= (BLUE SEP 1 84)
    0: 14110.4,    63: 14380.7,   119: 15695.5,   183:
15487.6,
  239: 15785.6,   295: 15921.7,   303: 15770.6,   359:
16043.7,
  423: 16228.7,   479: 16510.3,   543: 16845.7,   615:
17221.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 1, 1984 2.68 ppmC SYNURBAN, 0.97 ppmC MeOH (RED)
C:\PKSS\MECH\CALCHMN.PKS
CONC:
NO      =   0.252,
NO2     =   0.062,
ETHE    =   0.0804,
PRPE    =   0.0358,
TBUT    =   0.0132,
ALK4    =   0.2034,
ALK7    =   0.1377,
TOLU    =   0.0392,
XYLE    =   0.0256,
TMBZ    =   0.0086,
HCHO    =   0.037,
MEOH    =   0.9660,
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =           0.0043,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0184.lix;
TEMPERATURE= (SEP 1 84)
    0:  287.1,     59:  288.1,    123:  293.8,    179:  299.1,
  235:  302.8,    243:  303.1,    299:  305.4,    363:  307.1,
  419:  307.8,    483:  307.2,    539:  307.4,    613:  306.8;
WATER = (RED SEP 1 84)
    0: 8582.8,     59: 8716.7,    123: 8835.4,    179: 8946.9,
  243: 9007.5,    299: 9414.8,    355: 9333.8,    363: 9505.5,
  419: 9857.5,    483: 10038.0,   539: 10143.9,   613: 10448.0;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 1, 1984 2.68 ppmC SYNURBAN, 0.97 ppmC MeOH (RED)
C:\PKSS\MECH\CB42CHMN.PKS
CONC:
NO     =   0.252,
NO2    =   0.062,
ETH    =   0.0804,
OLE    =   0.0358,
PAR    =   1.7838,
TOL    =   0.0392,
XYL    =   0.0341,
HCHO   =   0.0370,
MEOH   =   0.9660,
RCHO   =   0.0202,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0043,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0184.LIX;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,   123:  293.8,   179:  299.1,
  235:  302.8,   243:  303.1,   299:  305.4,   363:  307.1,
  419:  307.8,   483:  307.2,   539:  307.4,   613:  306.8;
WATER = (RED SEP 1 84)
    0: 8582.8,    59: 8716.7,   123: 8835.4,   179: 8946.9,
  243: 9007.5,   299: 9414.8,   355: 9333.8,   363: 9505.5,
  419: 9857.5,   483: 10038.0,  539: 10143.9,  613: 10448.0;
DILUTION=
  0: 1 5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 1, 1984 3.26 ppmC SYNURBAN (BLUE)
C:\PKSS\MECH\CALCHMN.PKS
CONC:
NO   =              0.243,
NO2   =             0.059,
ETHE     =       0.1080,
PRPE     =       0.0509,
TBUT     =       0.0192,
ALK4     =       0.1427,
ALK7     =       0.1954,
TOLU     =       0.0590,
XYLE     =       0.0373,
TMBZ     =       0.0122,
HCHO     =       0.0550,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0041,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0184.LIX;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,   123:  293.8,   179:  299.1,
  235:  302.8,   243:  303.1,   299:  305.4,   363:  307.1,
  419:  307.8,   483:  307.2,   539:  307.4,   613:  306.8;
WATER= (BLUE SEP 1 84)
    0: 14110.4,    63: 14380.7,   119: 15695.5,   183:
15487.6,
  239: 15785.6,   295: 15921.7,   303: 15770.6,   359:
16043.7,
  423: 16228.7,   479: 16510.3,   543: 16845.7,   615:
17221.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 1, 1984 3.26 ppmC SYNURBAN (BLUE)
C:\PKSS\MECH\CB42CHMN.PKS
CONC:
NO    =   0.243,
NO2   =   0.059,
ETH   =   0.1080,
OLE   =   0.0509,
PAR   =   1.9587,
TOL   =   0.0590,
XYL   =   0.0495,
HCHO  =   0.0550,
RCHO  =   0.0299,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0041,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0184.lix;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,    123:  293.8,    179:  299.1,
  235:  302.8,   243:  303.1,    299:  305.4,    363:  307.1,
  419:  307.8,   483:  307.2,    539:  307.4,    613:  306.8;
WATER= (BLUE SEP 1 84)
    0: 14110.4,    63: 14380.7,   119: 15695.5,   183:
15487.6,
  239: 15785.6,   295: 15921.7,   303: 15770.6,   359:
16043.7,
  423: 16228.7,   479: 16510.3,   543: 16845.7,   615:
17221.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 1, 1984 2.68 ppmC SYNURBAN, 0.97 ppmC MeOH (RED)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO     =   0.252,
NO2    =   0.062,
ETH    =   0.0804,
OLE    =   0.0490,
ALK    =   0.3411,
AROM   =   0.0815,
HCHO   =   0.037,
MEOH   =   0.9660,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0043,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0184.lix;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,    123:  293.8,    179:  299.1,
  235:  302.8,   243:  303.1,    299:  305.4,    363:  307.1,
  419:  307.8,   483:  307.2,    539:  307.4,    613:  306.8;
EMISSIONS=2#
  0: 3.48E-3, 1.21E-5,
 59: 3.47E-3, 1.20E-5,
123: 3.40E-3, 1.16E-5,
179: 3.34E-3, 1.12E-5,
235: 3.30E-3, 1.09E-5,
243: 3.30E-3, 1.09E-5,
299: 3.27E-3, 1.07E-5,
363: 3.26E-3, 1.06E-5,
419: 3.25E-3, 1.06E-5,
483: 3.26E-3, 1.06E-5,
613: 3.28E-3, 1.06E-5;
WATER = (RED SEP 1 84)
    0: 8582.8,    59: 8716.7,    123: 8835.4,    179: 8946.9,
  243: 9007.5,   299: 9414.8,    355: 9333.8,    363: 9505.5,
  419: 9857.5,   483: 10038.0,   539: 10143.9,   613: 10448.0;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 1, 1984 2.68 ppmC SYNURBAN, 0.97 ppmC MeOH (RED)
C:\PKSS\mech\citchmw2.pks
CONC:
NO      =   0.252,
NO2     =   0.062,
ETH     =   0.0804,
OLE     =   0.0490,
ALK     =   0.3411,
AROM    =   0.0815,
HCHO    =   0.037,
MEOH    =   0.9660,
        (Surface NMHC = 0.0380 ppmC)
ALK    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
AROM   =   0.0007,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =            0.0043,
CO     =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0184.lix;
TEMPERATURE= (SEP 1 84)
    0:  287.1,     59:  288.1,    123:  293.8,    179:  299.1,
  235:  302.8,    243:  303.1,    299:  305.4,    363:  307.1,
  419:  307.8,    483:  307.2,    539:  307.4,    613:  306.8;
EMISSIONS=2#
   0: 3.48E-3, 1.21E-5,
  59: 3.47E-3, 1.20E-5,
 123: 3.40E-3, 1.16E-5,
 179: 3.34E-3, 1.12E-5,
 235: 3.30E-3, 1.09E-5,
 243: 3.30E-3, 1.09E-5,
 299: 3.27E-3, 1.07E-5,
 363: 3.26E-3, 1.06E-5,
 419: 3.25E-3, 1.06E-5,
 483: 3.26E-3, 1.06E-5,
 613: 3.26E-3, 1.06E-5;
WATER = (RED SEP 1 84)
    0: 8582.8,     59: 8716.7,    123: 8835.4,    179: 8946.9,
  243: 9007.5,    299: 9414.8,    355: 9333.8,    363: 9505.5,
  419: 9857.5,    483: 10038.0,   539: 10143.9,   613: 10448.0;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 1, 1984 3.26 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO   =              0.243,
NO2   =             0.059,
ETH     =        0.1080,
OLE     =        0.0701,
ALK     =        0.3381,
AROM    =        0.1213,
HCHO    =        0.0550,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0041,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0184.LIX;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,    123:  293.8,    179:  299.1,
  235:  302.8,   243:  303.1,    299:  305.4,    363:  307.1,
  419:  307.8,   483:  307.2,    539:  307.4,    613:  306.8;
EMISSIONS=2#
  0: 3.48E-3, 1.21E-5,
 59: 3.47E-3, 1.20E-5,
123: 3.40E-3, 1.16E-5,
179: 3.34E-3, 1.12E-5,
235: 3.30E-3, 1.09E-5,
243: 3.30E-3, 1.09E-5,
299: 3.27E-3, 1.07E-5,
363: 3.26E-3, 1.06E-5,
419: 3.25E-3, 1.06E-5,
483: 3.26E-3, 1.06E-5,
613: 3.26E-3, 1.06E-5;
WATER= (BLUE SEP 1 84)
    0: 14110.4,    63: 14380.7,   119: 15695.5,   183:
15487.6,
  239: 15785.6,   295: 15921.7,   303: 15770.6,   359:
16043.7,
  423: 16228.7,   479: 16510.3,   543: 16845.7,   615:
17221.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 1, 1984 3.26 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\citchmw2.pks
CONC:
NO    =               0.243,
NO2    =              0.059,
ETH      =         0.1080,
OLE      =         0.0701,
ALK      =         0.3381,
AROM     =         0.1213,
HCHO     =         0.0550,
       (Surface NMHC = 0.0380 ppmC)
ALK    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
AROM   =   0.0007,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =           0.0041,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0184.LIX;
TEMPERATURE= (SEP 1 84)
    0:  287.1,    59:  288.1,   123:  293.8,   179:  299.1,
  235:  302.8,   243:  303.1,   299:  305.4,   363:  307.1,
  419:  307.8,   483:  307.2,   539:  307.4,   613:  306.8;
EMISSIONS=2#
  0: 3.48E-3, 1.21E-5,
 59: 3.47E-3, 1.20E-5,
123: 3.40E-3, 1.16E-5,
179: 3.34E-3, 1.12E-5,
235: 3.30E-3, 1.09E-5,
243: 3.30E-3, 1.09E-5,
299: 3.27E-3, 1.07E-5,
363: 3.26E-3, 1.06E-5,
419: 3.25E-3, 1.06E-5,
483: 3.26E-3, 1.06E-5,
613: 3.26E-3, 1.06E-5;
WATER= (BLUE SEP 1 84)
    0: 14110.4,    63: 14380.7,   119: 15695.5,   183:
15487.6,
  239: 15785.6,   295: 15921.7,   303: 15770.6,   359:
16043.7,
  423: 16228.7,   479: 16510.3,   543: 16845.7,   615:
17221.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 2, 1984 1.24 ppmC SYNURBAN (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO    =                0.284,
NO2    =               0.060,
ETHE     =         0.0444,
PRPE     =         0.0211,
TBUT     =         0.0081,
ALK4     =         0.0519,
ALK7     =         0.0760,
TOLU     =         0.0190,
XYLE     =         0.0124,
TMBZ     =         0.0058,
HCHO     =         0.0184,
      (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =            0.0042,
CO     =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,TMBZ,
HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0284.lix;
TEMPERATURE= (SEP 2 84)
   0:  288.2,     58:  289.3,    114:  294.0,    122:  294.9,
178:  300.3,
 234:  304.4,   242:  305.2,    298:  307.5,    306:  307.6,
 354:  308.8,   362:  309.3,    418:  310.5,    426:  310.4,
474:  310.7,
 482:  310.8,   538:  310.9,    546:  311.0,    615:  310.0;
WATER= (RED SEP 2 84)
  0: 16151.0,    66: 17572.3,    114: 20281.4,    122: 20281.4,
178: 20400.6,
186: 20460.6,   234: 20420.6,    242: 20440.6,    298: 20702.3,
306: 20480.6,
354: 20804.0,   362: 20621.3,    418: 20824.3,    426: 20926.6,
474: 21153.7,
482: 21029.5,   538: 21510.3,    546: 21531.5,    594: 21510.3,
612: 21744.7;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 2, 1984 1.24 ppmC SYNURBAN (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =                  0.284,
NO2    =                 0.060,
ETH      =           0.0444,
OLE      =           0.0211,
PAR      =           0.7560,
TOL      =           0.0190,
XYL      =           0.0182,
HCHO     =           0.0184,
RCHO     =           0.0129,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0042,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=c:\pkss\lix\ST0284.lix;
TEMPERATURE= (SEP 2 84)
    0:  288.2,     58:  289.3,    114:  294.0,    122:  294.9,
178:  300.3,
  234:  304.4,   242:  305.2,    298:  307.5,    306:  307.6,
  354:  308.8,   362:  309.3,    418:  310.5,    426:  310.4,
474:  310.7,
  482:  310.8,   538:  310.9,    546:  311.0,    615:  310.0;
WATER= (RED SEP 2 84)
    0: 16151.0,     66: 17572.3,    114: 20281.4,    122:
20281.4,   178: 20400.6,
  186: 20460.6,   234: 20420.6,    242: 20440.6,    298:
20702.3,   306: 20480.6,
  354: 20804.0,   362: 20621.3,    418: 20824.3,    426:
20926.6,   474: 21153.7,
  482: 21029.5,   538: 21510.3,    546: 21531.5,    594:
21510.3,   612: 21744.7;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 2, 1984 0.90 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO    =              0.259,
NO2    =             0.063,
ETHE     =       0.0278,
PRPE     =       0.0144,
TBUT     =       0.0054,
ALK4     =       0.0539,
ALK7     =       0.0504,
TOLU     =       0.0129,
XYLE     =       0.0082,
TMBZ     =       0.0038,
HCHO     =       0.0121,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =            0.0044,
CO    =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0284.lix;
TEMPERATURE= (SEP 2 84)
    0:  288.2,    58:  289.3,   114:  294.0,   122:  294.9,
178:  300.3,
  234:  304.4,   242:  305.2,   298:  307.5,   306:  307.6,
  354:  308.8,   362:  309.3,   418:  310.5,   426:  310.4,
474:  310.7,
  482:  310.8,   538:  310.9,   546:  311.0,   615:  310.0;
WATER= (BLUE SEP 2 84)
    0: 16415.0,    62: 17106.0,   118: 18368.8,   174:
18333.4,
  182: 18404.3,   238: 18565.1,   246: 18457.7,   302:
18818.3,
  358: 19093.9,   366: 18873.0,   422: 19205.3,   478:
19620.3,
  486: 19582.1,   534: 19716.0,   542: 19967.2,   606:
20025.7;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 2, 1984 0.90 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =              0.259,
NO2    =             0.063,
ETH     =        0.0278,
OLE     =        0.0144,
PAR     =        0.5816,
TOL     =        0.0129,
XYL     =        0.0119,
HCHO    =        0.0121,
RCHO    =        0.0085,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0044,
CO    =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0284.lix;
TEMPERATURE= (SEP 2 84)
     0:  288.2,    58:  289.3,   114:  294.0,   122:  294.9,
178:  300.3,
   234:  304.4,   242:  305.2,   298:  307.5,   306:  307.6,
   354:  308.8,   362:  309.3,   418:  310.5,   426:  310.4,
474:  310.7,
   482:  310.8,   538:  310.9,   546:  311.0,   615:  310.0;
WATER= (BLUE SEP 2 84)
    0: 16415.0,    62: 17106.0,   118: 18368.8,   174:
18333.4,
   182: 18404.3,   238: 18565.1,   246: 18457.7,   302:
18818.3,
   358: 19093.9,   366: 18873.0,   422: 19205.3,   478:
19620.3,
   486: 19582.1,   534: 19716.0,   542: 19967.2,   606:
20025.7;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 2, 1984 1.24 ppmC SYNURBAN (RED)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO    =              0.284,
NO2    =             0.060,
ETH     =        0.0444,
OLE     =        0.0292,
ALK     =        0.1279,
AROM    =        0.0423,
HCHO     =        0.0184,
       (Surface NMHC = 0.0380 ppmC)
ALK    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
AROM   =   0.0007,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =            0.0042,
CO     =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0284.lix;
TEMPERATURE= (SEP 2 84)
   0:  288.2,     58:  289.3,    114:  294.0,    122:  294.9,
178:  300.3,
 234:  304.4,   242:  305.2,    298:  307.5,    306:  307.6,
 354:  308.8,   362:  309.3,    418:  310.5,    426:  310.4,
474:  310.7,
 482:  310.8,   538:  310.9,    546:  311.0,    615:  310.0;
EMISSIONS=2#
   0: 3.45E-3, 1.20E-5,  58: 3.46E-3, 1.19E-5,
 114: 3.40E-3, 1.17E-5, 122: 3.39E-3, 1.15E-5,
 178: 3.33E-3, 1.11E-5, 234: 3.29E-3, 1.08E-5,
 242: 3.28E-3, 1.07E-5, 298: 3.25E-3, 1.06E-5,
 306: 3.25E-3, 1.06E-5, 354: 3.24E-3, 1.05E-5,
 362: 3.23E-3, 1.04E-5, 418: 3.22E-3, 1.04E-5,
 546: 3.22E-3, 1.03E-5, 615: 3.23E-3, 1.04E-5;
WATER= (RED SEP 2 84)
  0: 16151.0,    66: 17572.3,   114: 20281.4,   122: 20281.4,
178: 20400.6,
186: 20460.6,   234: 20420.6,   242: 20440.6,   298: 20702.3,
306: 20480.6,
354: 20804.0,   362: 20621.3,   418: 20824.3,   426: 20926.6,
474: 21153.7,
482: 21029.5,   538: 21510.3,   546: 21531.5,   594: 21510.3,
612: 21744.7;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 2, 1984 1.24 ppmC SYNURBAN (RED)
C:\PKSS\mech\citchmw2.pks
CONC:
NO    =                0.284,
NO2    =               0.060,
ETH     =         0.0444,
OLE     =         0.0292,
ALK     =         0.1279,
AROM    =         0.0423,
HCHO     =         0.0184,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =              0.0042,
CO    =              0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0284.lix;
TEMPERATURE= (SEP 2 84)
   0:  288.2,     58:  289.3,    114:  294.0,    122:  294.9,
178:  300.3,
 234:  304.4,   242:  305.2,    298:  307.5,    306:  307.6,
 354:  308.8,   362:  309.3,    418:  310.5,    426:  310.4,
474:  310.7,
 482:  310.8,   538:  310.9,    546:  311.0,    615:  310.0;
EMISSIONS=2#
  0: 3.45E-3, 1.20E-5,  58: 3.46E-3, 1.19E-5,
114: 3.40E-3, 1.17E-5, 122: 3.39E-3, 1.15E-5,
178: 3.33E-3, 1.11E-5, 234: 3.29E-3, 1.08E-5,
242: 3.28E-3, 1.07E-5, 298: 3.25E-3, 1.06E-5,
306: 3.25E-3, 1.06E-5, 354: 3.24E-3, 1.05E-5,
362: 3.23E-3, 1.04E-5, 418: 3.22E-3, 1.04E-5,
546: 3.22E-3, 1.03E-5, 615: 3.23E-3, 1.04E-5;
WATER= (RED SEP 2 84)
  0: 16151.0,    66: 17572.3,    114: 20281.4,    122: 20281.4,
178: 20400.6,
186: 20460.6,   234: 20420.6,    242: 20440.6,    298: 20702.3,
306: 20480.6,
354: 20804.0,   362: 20621.3,    418: 20824.3,    426: 20926.6,
474: 21153.7,
482: 21029.5,   538: 21510.3,    546: 21531.5,    594: 21510.3,
612: 21744.7;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 2, 1984 0.90 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO    =            0.259,
NO2   =            0.063,
ETH     =       0.0278,
OLE     =       0.0198,
ALK     =       0.1043,
AROM    =       0.0282,
HCHO    =       0.0121,
        (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0044,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0284.lix;
TEMPERATURE= (SEP 2 84)
    0:  288.2,    58:  289.3,    114:  294.0,    122:  294.9,
178:  300.3,
  234:  304.4,   242:  305.2,    298:  307.5,    306:  307.6,
  354:  308.8,   362:  309.3,    418:  310.5,    426:  310.4,
474:  310.7,
  482:  310.8,   538:  310.9,    546:  311.0,    615:  310.0;
EMISSIONS=2#
  0: 3.45E-3, 1.20E-5,  58: 3.46E-3, 1.19E-5,
114: 3.40E-3, 1.17E-5, 122: 3.39E-3, 1.15E-5,
178: 3.33E-3, 1.11E-5, 234: 3.29E-3, 1.08E-5,
242: 3.28E-3, 1.07E-5, 298: 3.25E-3, 1.06E-5,
306: 3.25E-3, 1.06E-5, 354: 3.24E-3, 1.05E-5,
362: 3.23E-3, 1.04E-5, 418: 3.22E-3, 1.04E-5,
546: 3.22E-3, 1.03E-5, 615: 3.23E-3, 1.04E-5;
WATER= (BLUE SEP 2 84)
    0: 16415.0,    62: 17106.0,   118: 18368.8,   174:
18333.4,
  182: 18404.3,   238: 18565.1,   246: 18457.7,   302:
18818.3,
  358: 19093.9,   366: 18873.0,   422: 19205.3,   478:
19620.3,
  486: 19582.1,   534: 19716.0,   542: 19967.2,   606:
20025.7;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 2, 1984 0.90 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\citchmw2.pks
CONC:
NO    =               0.259,
NO2    =              0.063,
ETH      =        0.0278,
OLE      =        0.0198,
ALK      =        0.1043,
AROM     =        0.0282,
HCHO     =        0.0121,
       (Surface NMHC = 0.0380 ppmC)
ALK    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
AROM   =   0.0007,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =           0.0044,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0284.lix;
TEMPERATURE= (SEP 2 84)
    0:  288.2,    58:  289.3,   114:  294.0,   122:  294.9,
178:  300.3,
  234:  304.4,   242:  305.2,   298:  307.5,   306:  307.6,
  354:  308.8,   362:  309.3,   418:  310.5,   426:  310.4,
474:  310.7,
  482:  310.8,   538:  310.9,   546:  311.0,   615:  310.0;
EMISSIONS=2#
  0: 3.45E-3, 1.20E-5,  58: 3.46E-3, 1.19E-5,
114: 3.40E-3, 1.17E-5, 122: 3.39E-3, 1.15E-5,
178: 3.33E-3, 1.11E-5, 234: 3.29E-3, 1.08E-5,
242: 3.28E-3, 1.07E-5, 298: 3.25E-3, 1.06E-5,
306: 3.25E-3, 1.06E-5, 354: 3.24E-3, 1.05E-5,
362: 3.23E-3, 1.04E-5, 418: 3.22E-3, 1.04E-5,
546: 3.22E-3, 1.03E-5, 615: 3.23E-3, 1.04E-5;
WATER= (BLUE SEP 2 84)
    0: 18415.0,    62: 17106.0,   118: 18368.8,   174:
18333.4,
  182: 18404.3,   238: 18565.1,   246: 18457.7,   302:
18818.3,
  358: 19093.9,   366: 18873.0,   422: 19205.3,   478:
19620.3,
  486: 19582.1,   534: 19716.0,   542: 19967.2,   606:
20025.7;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 3, 1984 1.09 ppmC SYNURBAN (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO   =              0.241,
NO2    =            0.111,
ETHE     =        0.0402,
PRPE     =        0.0156,
TBUT     =        0.0061,
ALK4     =        0.0470,
ALK7     =        0.0644,
TOLU     =        0.0195,
XYLE     =        0.0127,
TMBZ     =        0.0053,
HCHO     =        0.0186,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =           0.0078,
CO    =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0384.LIX;
TEMPERATURE=   (SEPT 2, 1984)
   0 : 288.2 ,  61 : 289.6 , 125 : 295.5 , 181 :   301 , 245 :
305.6 ,
 301 : 307.6 , 365 : 309.3 , 421 : 310.4 , 485 : 310.9 , 541 :
311 ,
 605 : 309.8 ;
WATER= (SEPT 2, 1984)
   0 : 16151.3 ,  61 : 17572.3 , 125 : 20301.2 , 181 : 20460.6
,
 245 : 20460.6 , 301 : 20480.6 , 365 : 20844.7 , 421 : 20926.6
,
 485 : 21153.7 , 541 : 21531.5 , 605 : 21616.5 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
September 3, 1984 1.09 ppmC SYNURBAN (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO   =              0.241,
NO2   =             0.111,
ETH      =        0.0402,
OLE      =        0.0156,
PAR      =        0.6524,
TOL      =        0.0195,
XYL      =        0.0180,
HCHO     =        0.0186,
RCHO     =        0.0094,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0078,
CO     =             0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0384.LIX;
TEMPERATURE=   (SEP 2, 1984)
   0 : 288.2 ,  61 : 289.6 , 125 : 295.5 , 181 :   301 , 245 :
305.6 ,
 301 : 307.6 , 365 : 309.3 , 421 : 310.4 , 485 : 310.9 , 541 :
311 ,
 605 : 309.8 ;
WATER= (RED)    (SEP 2, 1984)
   0 : 16151.3 ,  61 : 17572.3 , 125 : 20301.2 , 181 : 20460.6
,
 245 : 20460.6 , 301 : 20480.6 , 365 : 20844.7 , 421 : 20926.6
,
 485 : 21153.7 , 541 : 21531.5 , 605 : 21616.5 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 3, 1984 0.79 ppmC SYNURBAN, 0.26 ppmC MeOH, 0.06
ppmC HCHO (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO   =              0.240,
NO2   =             0.112,
ETHE     =        0.0301,
PRPE     =        0.0124,
TBUT     =        0.0041,
ALK4     =        0.0325,
ALK7     =        0.0471,
TOLU     =        0.0140,
XYLE     =        0.0092,
TMBZ     =        0.0039,
HCHO     =        0.0744,
MEOH   =    0.2643,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0078,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0384.LIX;
TEMPERATURE=   (SEPT. 2, 1984)
   0 : 288.2 ,  61 : 289.6 , 125 : 295.5 , 181 :   301 , 245 :
305.6 ,
 301 : 307.6 , 365 : 309.3 , 421 : 310.4 , 485 : 310.9 , 541 :
311 ,
 605 : 309.8 ;
WATER= (SEPT. 2, 1984)
   0 : 17337.5 ,  65 : 17337.5 , 121 : 18457.7 , 185 : 18351.1
,
 241 : 18457.7 , 297 : 18818.3 , 361 :   18873 , 425 : 19112.4
,
 489 : 19544.1 , 545 : 19735.1 , 601 : 20025.7 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 3, 1984 0.79 ppmC SYNURBAN, 0.26 ppmC MeOH (BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO   =                0.240,
NO2   =               0.112,
ETH      =         0.0301,
OLE      =         0.0124,
PAR      =         0.4682,
TOL      =         0.0140,
XYL      =         0.0131,
HCHO     =         0.0744,
RCHO     =         0.0062,
MEOH     =         0.2643,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0078,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0384.LIX;
TEMPERATURE=   (SEP 2, 1984)
   0 : 288.2 ,  61 : 289.6 , 125 : 295.5 , 181 :   301 , 245 :
305.6 ,
 301 : 307.6 , 365 : 309.3 , 421 : 310.4 , 485 : 310.9 , 541 :
311 ,
 605 : 309.8 ;
WATER= (BLUE)    (SEP 2, 1984)
   0 : 17337.5 ,  65 : 17337.5 , 121 : 18457.7 , 185 : 18351.1
,
 241 : 18457.7 , 297 : 18818.3 , 361 :   18873 , 425 : 19112.4
,
 489 : 19544.1 , 545 : 19735.1 , 601 : 20025.7 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 3, 1984 1.09 ppmC SYNURBAN (RED)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO   =              0.241,
NO2   =             0.111,
ETH     =        0.0402,
OLE     =        0.0271,
ALK     =        0.1114,
AROM    =        0.0427,
HCHO    =        0.0186,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   .          0.0078,
CO    =              0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0384.LIX;
TEMPERATURE=   (SEPT 2, 1984)
   0 : 288.2 ,  61 : 289.6 , 125 : 295.5 , 181 :   301 , 245 :
305.6 ,
 301 : 307.6 , 365 : 309.3 , 421 : 310.4 , 485 : 310.9 , 541 :
311 ,
 605 : 309.8 ;
EMISSIONS=2#
  0: 3.47E-3, 1.20E-5,
 61: 3.45E-3, 1.19E-5,
125: 3.38E-3, 1.14E-5,
181: 3.32E-3, 1.10E-5,
245: 3.27E-3, 1.07E-5,
301: 3.25E-3, 1.06E-5,
365: 3.23E-3, 1.04E-5,
421: 3.22E-3, 1.04E-5,
485: 3.22E-3, 1.03E-5,
541: 3.22E-3, 1.03E-5,
605: 3.23E-3, 1.04E-5;
WATER= (SEPT 2, 1984)
   0 : 16151.3 ,  61 : 17572.3 , 125 : 20301.2 , 181 : 20460.6
,
 245 : 20460.6 , 301 : 20480.6 , 365 : 20844.7 , 421 : 20926.6
,
 485 : 21153.7 , 541 : 21531.5 , 605 : 21616.5 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 3, 1984 1.09 ppmC SYNURBAN (RED)
C:\PKSS\mech\citchmw2.pks
CONC:
NO   =              0.241,
NO2   =             0.111,
ETH     =        0.0402,
OLE     =        0.0271,
ALK     =        0.1114,
AROM    =        0.0427,
HCHO    =        0.0186,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0078,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0384.LIX;
TEMPERATURE=   (SEPT 2, 1984)
   0 : 288.2 ,  61 : 289.6 , 125 : 295.5 , 181 :   301 , 245 :
305.6 ,
 301 : 307.6 , 365 : 309.3 , 421 : 310.4 , 485 : 310.9 , 541 :
311, ,
 605 : 309.8 ;
EMISSIONS=2#
  0: 3.47E-3, 1.20E-5,
 61: 3.45E-3, 1.19E-5,
125: 3.38E-3, 1.14E-5,
181: 3.32E-3, 1.10E-5,
245: 3.27E-3, 1.07E-5,
301: 3.25E-3, 1.06E-5,
365: 3.23E-3, 1.04E-5,
421: 3.22E-3, 1.04E-5,
485: 3.22E-3, 1.03E-5,
541: 3.22E-3, 1.03E-5,
605: 3.23E-3, 1.04E-5;
WATER= (SEPT 2, 1984)
   0 : 16151.3 ,  61 : 17572.3 , 125 : 20301.2 , 181 : 20460.6
,
 245 : 20460.6 , 301 : 20480.6 , 365 : 20844.7 , 421 : 20926.6
,
 485 : 21153.7 , 541 : 21531.5 , 605 : 21616.5 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 3, 1984 0.79 ppmC SYNURBAN, 0.26 ppmC MeOH, 0.06
ppmC HCHO (BLUE)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO   =              0.240,
NO2   =             0.112,
ETH     =        0.0301,
OLE     =        0.0165,
ALK     =        0.0796,
AROM    =        0.0316,
HCHO    =        0.0744,
MEOH   =    0.2643,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0078,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0384.LIX;
TEMPERATURE=   (SEPT. 2, 1984)
   0 : 288.2 ,  61 : 289.6 , 125 : 295.5 , 181 :   301 , 245 :
305.6 ,
 301 : 307.6 , 365 : 309.3 , 421 : 310.4 , 485 : 310.9 , 541 :
311 ,
 605 : 309.8 ;
EMISSIONS=2#
  0: 3.47E-3, 1.20E-5,
 61: 3.45E-3, 1.19E-5,
125: 3.38E-3, 1.14E-5,
181: 3.32E-3, 1.10E-5,
245: 3.27E-3, 1.07E-5,
301: 3.25E-3, 1.06E-5,
365: 3.23E-3, 1.04E-5,
421: 3.22E-3, 1.04E-5,
485: 3.22E-3, 1.03E-5,
541: 3.22E-3, 1.03E-5,
605: 3.23E-3, 1.04E-5;
WATER= (SEPT. 2, 1984)
   0 : 17337.5 ,  65 : 17337.5 , 121 : 18457.7 , 185 : 18351.1
,
 241 : 18457.7 , 297 : 18818.3 , 361 :   18873 , 425 : 19112.4
,
 489 : 19544.1 , 545 : 19735.1 , 601 : 20025.7 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 3, 1984 0.79 ppmC SYNURBAN, 0.26 ppmC MeOH, 0.06
ppmC HCHO (BLUE)
C:\PKSS\mech\citchmw2.pks
CONC:
NO    =                0.240,
NO2    =               0.112,
ETH      =         0.0301,
OLE      =         0.0165,
ALK      =         0.0796,
AROM     =         0.0316,
HCHO     =         0.0744,
MEOH    =    0.2643,
          (Surface NMHC = 0.0380 ppmC)
ALK    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
AROM   =   0.0007,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =             0.0078,
CO     =             0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0384.LIX;
TEMPERATURE=   (SEPT. 2, 1984)
   0 : 288.2 ,  61 : 289.6 , 125 : 295.5 , 181 :   301 , 245 :
305.6 ,
 301 : 307.6 , 365 : 309.3 , 421 : 310.4 , 485 : 310.9 , 541 :
311 ,
 605 : 309.8 ;
EMISSIONS=2#
  0: 3.47E-3, 1.20E-5,
 61: 3.45E-3, 1.19E-5,
125: 3.38E-3, 1.14E-5,
181: 3.32E-3, 1.10E-5,
245: 3.27E-3, 1.07E-5,
301: 3.25E-3, 1.06E-5,
365: 3.23E-3, 1.04E-5,
421: 3.22E-3, 1.04E-5,
485: 3.22E-3, 1.03E-5,
541: 3.22E-3, 1.03E-5,
605: 3.23E-3, 1.04E-5;
WATER= (SEPT. 2, 1984)
   0 : 17337.5 ,  65 : 17337.5 . 121 : 18457.7 , 185 : 18351.1
,
 241 : 18457.7 , 297 : 18818.3 , 361 :   18873 , 425 : 19112.4
,
 489 : 19544.1 , 545 : 19735.1 , 601 : 20025.7 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 8, 1984, 1.8 ppmC SynAuto (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =        0.223,
NO2     =        0.119,
ALK4    =        0.105,
ALK7    =        0.018,
ETHE    =        0.320,
PRPE    =        0.040,
TBUT    =        0.010,
TOLU    =        0.033,
XYLE    =        0.022,
TMBZ    =        0.007,
HCHO    =        0.036,
(NROG   =        0.004,
 MISS   =        0.018)
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0083,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0884.lIx;
TEMPERATURE= (ST 8 84)
    0:  281.6,    30:  281.5,    60:  282.0,    120:  289.0,
  180:  295.0,   240:  299.0,   300:  302.0,    360:  303.7,
  420:  304.1,   480:  304.3,   540:  304.3,    600:  303.7;
WATER= (RED ST 8 84)
    5: 6074.6,   29: 6087.1,   69: 6112.1,   125: 6206.6,
  181: 6187.6,  237: 6399.2,  301: 6670.0,   359: 6874.1,
  421: 7196.9,  477: 7532.2,  549: 7965.9,   597: 8258.8;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 8, 1984, 1.8 ppmC SynAuto (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO   =            0.223,
NO2   =           0.119,
PAR     =         0.633,
ETH     =         0.320,
OLE     =         0.040,
TOL     =         0.033,
XYL     =         0.029,
HCHO    =         0.036,
RCHO    =         0.021,
(NR     =         0.030,)
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0083,
CO    =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\st0884.lIx;
TEMPERATURE= (ST 8 84)
    0:  281.6,    30:  281.5,    60:  282.0,   120:  289.0,
  180:  295.0,   240:  299.0,   300:  302.0,   360:  303.7,
  420:  304.1,   480:  304.3,   540:  304.3,   600:  303.7;
WATER= (RED ST 8 84)
    5: 6074.6,   29: 6087.1,   69: 6112.1,  125: 6206.6,
  181: 6187.6,  237: 6399.2,  301: 6670.0,  359: 6874.1,
  421: 7196.9,  477: 7532.2,  549: 7965.9,  597: 8258.8;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 8, 1984, 2.8 ppmC SynAuto (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =         0.205,
NO2     =         0.128,
ALK4    =         0.154,
ALK7    =         0.030,
ETHE    =         0.490,
PRPE    =         0.063,
TBUT    =         0.014,
TOLU    =         0.040,
XYLE    =         0.030,
TMBZ    =         0.011,
HCHO    =         0.054,
(NROG   =         0.005,
 MISS   =         0.037)
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =           0.0090,
CO      =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST0884.lIx;
TEMPERATURE= (ST 8 84)
    0:  281.6,    30:  281.5,    60:  282.0,   120:  289.0,
  180:  295.0,   240:  299.0,   300:  302.0,   360:  303.7,
  420:  304.1,   480:  304.3,   540:  304.3,   600:  303.7;
WATER= (BLUE ST 8 84)
    9: 7428.8,   33: 7458.2,  121: 7539.6,  185: 7606.8,
  257: 7735.0,  305: 7919.3,  361: 8234.7,  417: 8536.1,
  481: 8821.6,  529: 9221.4,  593: 9637.4;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 8, 1984, 2.8 ppmC SynAuto (BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =            0.205,
NO2    =           0.128,
PAR      =         0.980,
ETH      =         0.490,
OLE      =         0.063,
TOL      =         0.040,
XYL      =         0.041,
HCHO     =         0.054,
RCHO     =         0.028,
(NR      =         0.039,)
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0090,
CO    =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST0884.lIx;
TEMPERATURE= (ST 8 84)
    0:  281.6,    30:  281.5,    60:  282.0,   120:  289.0,
  180:  295.0,   240:  299.0,   300:  302.0,   360:  303.7,
  420:  304.1,   480:  304.3,   540:  304.3,   600:  303.7;
WATER= (BLUE ST 8 84)
    9: 7428.8,   33: 7458.2,  121: 7539.6,  185: 7606.8,
  257: 7735.0,  305: 7919.3,  361: 8234.7,  417: 8536.1,
  481: 8821.6,  529: 9221.4,  593: 9637.4;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 17, 1984, 2.18 ppmC SynAuto (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO     =         0.272,
NO2    =         0.069,
ALK4   =         0.052,
ALK7   =         0.031,
ETHE   =         0.286,
PRPE   =         0.052,
TBUT   =         0.014,
TOLU   =         0.062,
XYLE   =         0.039,
TMBZ   =         0.013,
HCHO   =         0.036,
(NROG  =         0.007,
 MISS  =         0.078)
       (Surface NMHC = 0.0380 ppmC)
ALK4   =    0.0201,
ETHE   =    0.0009,
PRPE   =    0.0006,
TOLU   =    0.0004,
XYLE   =    0.0003,
HCHO   =    0.0038,
ALD2   =    0.0030,
HONO   =             0.0048,
CO     =             0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST1784.lIx;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,   120:  287.5,
  180:  292.5,   240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,   480:  298.9,   540:  298.6,   600:  297.5;
WATER= (RED ST 19 84)
    0: 9500.0,   60: 9500.0,  164: 15744.7, 196: 16801.1,
  236: 17126.1, 308: 17175.5, 380: 17407.7, 420: 17592.6,
  476: 17728.5, 564: 18090.4, 596: 17917.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 17, 1984, 2.18 ppmC SynAuto (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO   =            0.272,
NO2   =           0.069,
PAR      =        0.548,
ETH      =        0.286,
OLE      =        0.052,
TOL      =        0.062,
XYL      =        0.052,
HCHO     =        0.036,
RCHO     =        0.028,
(NR      =        0.052,)
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0048,
CO    =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\st1784.lIx;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,   120:  287.5,
  180:  292.5,   240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,   480:  298.9,   540:  298.6,   600:  297.5;
WATER= (RED ST 19 84)
    0: 9500.0,   60: 9500.0,  164: 15744.7, 196: 16801.1,
  236: 17126.1, 308: 17175.5, 380: 17407.7, 420: 17592.6,
  476: 17728.5, 564: 18090.4, 596: 17917.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 17, 1984, 1/3 MEOH W/10% HCHO (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =         0.272,
NO2     =         0.068,
ALK4    =         0.031,
ALK7    =         0.021,
ETHE    =         0.192,
PRPE    =         0.036,
TBUT    =         0.009,
TOLU    =         0.040,
XYLE    =         0.028,
TMBZ    =         0.009,
HCHO    =         0.083,
MEOH    =         0.571,
(NROG   =         0.006,
 MISS   =         0.056)
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0048,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST1784.lIx;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,   120:  287.5,
  180:  292.5,   240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,   480:  298.9,   540:  298.6,   600:  297.5;
WATER= (BLUE ST 19 84)
    0: 9500.0,   60: 9500.0,  168: 12408.7,  240: 12350.1,
  312: 12973.4, 360: 13499.8, 424: 13680.0,  480: 13758.0,
  544: 13889.0, 600: 14128.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 17, 1984, 1/3 MEOH W/10% HCHO (BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =            0.272,
NO2    =           0.068,
PAR      =         0.353,
ETH      =         0.192,
OLE      =         0.036,
TOL      =         0.040,
XYL      =         0.036,
HCHO     =         0.083,
RCHO     =         0.018,
MEOH     =         0.571,
(NR      =         0.042,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0048,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST1784.lIx;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,   120:  287.5,
  180:  292.5,   240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,   480:  298.9,   540:  298.6,   600:  297.5;
WATER= (BLUE ST 19 84)
    0: 9500.0,   60: 9500.0,  168: 12408.7,  240: 12350.1,
  312: 12973.4, 360: 13499.8, 424: 13680.0,  480: 13758.0,
  544: 13889.0, 600: 14128.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 17, 1984, 2.18 ppmC SynAuto (RED)
C:\PKSS\MECH\CALCHMK.PKS
CONC:
NO      =       0.272,
NO2     =       0.069,
ALK4    =       0.052,
ALK7    =       0.031,
ETHE    =       0.286,
PRPE    =       0.052,
TBUT    =       0.014,
TOLU    =       0.062,
XYLE    =       0.039,
TMBZ    =       0.013,
HCHO    =       0.036,
(NROG   =       0.007,
 MISS   =       0.078)
        (Surface NMHC = 0.0380 ppmC)
ALK4    =  0.0201,
ETHE    =  0.0009,
PRPE    =  0.0006,
TOLU    =  0.0004,
XYLE    =  0.0003,
HCHO    =  0.0038,
ALD2    =  0.0030,
HONO    =         0.0048,
CO      =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST1784.1Ix;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,   120:  287.5,
  180:  292.5,   240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,   480:  298.9,   540:  298.6,   600:  297.5;
WATER= (RED ST 19 84)
    0: 9500.0,   60: 9500.0,  164: 15744.7, 196: 16801.1,
  236: 17126.1, 308: 17175.5, 380: 17407.7, 420: 17592.6,
  476: 17728.5, 564: 18090.4, 596: 17917.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 17, 1984, 2.18 ppmC SynAuto (RED)
C:\PKSS\MECH\CB42CHMK.PKS
CONC:
NO   =          0.272,
NO2   =         0.069,
PAR     =       0.548,
ETH     =       0.286,
OLE     =       0.052,
TOL     =       0.062,
XYL     =       0.052,
HCHO    =       0.036,
RCHO    =       0.028,
(NR     =       0.052,)
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0048,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\st1784.lIx;
TEMPERATURE= (ST 17 84)
    0:  280.0,   60:  280.5,   120:  287.5,
  180:  292.5,  240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,  480:  298.9,   540:  298.6,   600:  297.5;
WATER= (RED ST 19 84)
    0: 9500.0,   60: 9500.0,  164: 15744.7, 196: 16801.1,
  236: 17126.1, 308: 17175.5, 380: 17407.7, 420: 17592.6,
  476: 17728.5, 564: 18090.4, 596: 17917.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 17, 1984, 1/3 MEOH W/10% HCHO (BLUE)
C:\PKSS\MECH\CALCHMK.PKS
CONC:
NO      =        0.272,
NO2     =        0.068,
ALK4    =        0.031,
ALK7    =        0.021,
ETHE    =        0.192,
PRPE    =        0.036,
TBUT    =        0.009,
TOLU    =        0.040,
XYLE    =        0.028,
TMBZ    =        0.009,
HCHO    =        0.083,
MEOH    =        0.571,
(NROG   =        0.006,
 MISS   =        0.056)
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0048,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST1784.1Ix;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,   120:  287.5,
  180:  292.5,   240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,   480:  298.9,   540:  298.6,   600:  297.5;
WATER= (BLUE ST 19 84)
    0: 9500.0,   60: 9500.0,  168: 12408.7,  240: 12350.1,
  312: 12973.4, 360: 13499.8, 424: 13680.0,  480: 13758.0,
  544: 13889.0, 600: 14128.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 17, 1984, 1/3 MEOH W/10% HCHO (BLUE)
C:\PKSS\MECH\CB42CHMK.PKS
CONC:
NO   =          0.272,
NO2   =         0.068,
PAR     =       0.353,
ETH     =       0.192,
OLE     =       0.036,
TOL     =       0.040,
XYL     =       0.036,
HCHO    =       0.083,
RCHO    =       0.018,
MEOH    =       0.571,
(NR     =       0.042,)
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0048,
CO    =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST1784.lIx;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,   120:  287.5,
  180:  292.5,   240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,   480:  298.9,   540:  298.6,   600:  297.5;
WATER= (BLUE ST 19 84)
    0: 9500.0,   60: 9500.0,  168: 12408.7,  240: 12350.1,
  312: 12973.4, 360: 13499.8, 424: 13680.0,  480: 13758.0,
  544: 13889.0, 600: 14128.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 17, 1984, 2.18 ppmC SynAuto (RED)
C:\PKSS\MECH\CALCHMN.PKS
CONC:
NO      =        0.272,
NO2     =        0.069,
ALK4    =        0.052,
ALK7    =        0.031,
ETHE    =        0.286,
PRPE    =        0.052,
TBUT    =        0.014,
TOLU    =        0.062,
XYLE    =        0.039,
TMBZ    =        0.013,
HCHO    =        0.036,
(NROG   =        0.007,
 MISS   =        0.078)
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =            0.0048,
CO      =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST1784.lIx;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,    120:  287.5,
  180:  292.5,   240:  296.0,    300:  296.5,    360:  299.0,
  420:  299.4,   480:  298.9,    540:  298.6,    600:  297.5;
WATER= (RED ST 19 84)
    0: 9500.0,   60: 9500.0,  164: 15744.7, 196: 16801.1,
  236: 17126.1, 308: 17175.5, 380: 17407.7, 420: 17592.6,
  476: 17728.5, 564: 18090.4, 596: 17917.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 17, 1984, 2.18 ppmC SynAuto (RED)
C:\PKSS\MECH\CB42CHMN.PKS
CONC:
NO    =           0.272,
NO2    =          0.069,
PAR      =        0.548,
ETH      =        0.286,
OLE      =        0.052,
TOL      =        0.062,
XYL      =        0.052,
HCHO     =        0.036,
RCHO     =        0.028,
(NR      =        0.052,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0048,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\st1784.lIx;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,   120:  287.5,
  180:  292.5,   240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,   480:  298.9,   540:  298.6,   600:  297.5;
WATER= (RED ST 19 84)
    0: 9500.0,   60: 9500.0,  164: 15744.7, 196: 16801.1,
  236: 17126.1, 308: 17175.5, 380: 17407.7, 420: 17592.6,
  476: 17728.5, 564: 18090.4, 596: 17917.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 17, 1984, 1/3 MEOH W/10% HCHO (BLUE)
C:\PKSS\MECH\CALCHMN.PKS
CONC:
NO      =         0.272,
NO2     =         0.068,
ALK4    =         0.031,
ALK7    =         0.021,
ETHE    =         0.192,
PRPE    =         0.036,
TBUT    =         0.009,
TOLU    =         0.040,
XYLE    =         0.028,
TMBZ    =         0.009,
HCHO    =         0.083,
MEOH    =         0.571,
(NROG   =         0.006,
 MISS   =         0.056)
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0048,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST1784.lIx;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,   120:  287.5,
  180:  292.5,   240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,   480:  298.9,   540:  298.6,   600:  297.5;
WATER= (BLUE ST 19 84)
    0: 9500.0,   60: 9500.0,  168: 12408.7,  240: 12350.1,
  312: 12973.4, 360: 13499.8, 424: 13680.0,  480: 13758.0,
  544: 13889.0, 600: 14128.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=            600;
FINISH
!
```

```
September 17, 1984, 1/3 MEOH W/10% HCHO (BLUE)
C:\PKSS\MECH\CB42CHMN.PKS
CONC:
NO    =            0.272,
NO2    =           0.068,
PAR      =         0.353,
ETH      =         0.192,
OLE      =         0.036,
TOL      =         0.040,
XYL      =         0.036,
HCHO     =         0.083,
RCHO     =         0.018,
MEOH     =         0.571,
(NR      =         0.042,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0048,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST1784.lIx;
TEMPERATURE= (ST 17 84)
    0:  280.0,    60:  280.5,   120:  287.5,
  180:  292.5,   240:  296.0,   300:  296.5,   360:  299.0,
  420:  299.4,   480:  298.9,   540:  298.6,   600:  297.5;
WATER= (BLUE ST 19 84)
    0: 9500.0,   60: 9500.0,  168: 12408.7,  240: 12350.1,
  312: 12973.4, 360: 13499.8, 424: 13680.0,  480: 13758.0,
  544: 13889.0, 600: 14128.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 19, 1984, 4.4 ppmC HMW SynAuto (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO       =        0.254,
NO2      =        0.085,
ALK7     =        0.118,
TOLU     =        0.228,
XYLE     =        0.148,
TMBZ     =        0.056,
(NROG    =        0.030,
 MISS    =        0.241)
        (Surface NMHC = 0.0380 ppmC)
ALK4     =   0.0201,
ETHE     =   0.0009,
PRPE     =   0.0006,
TOLU     =   0.0004,
XYLE     =   0.0003,
HCHO     =   0.0038,
ALD2     =   0.0030,
HONO     =            0.0060,
CO       =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST1984.lIx;
TEMPERATURE= (ST 19 84)
    0:  280.3,    60:  280.9,    120:  287.4,
  180:  291.9,   240:  297.2,    300:  298.9,    360:  300.7,
  420:  301.4,   480:  301.9,    540:  301.8,    600:  300.0;
WATER= (RED ST 19 84)
    0: 9500.0,    60: 9500.0,  164: 15744.7, 196: 16801.1,
  236: 17126.1, 308: 17175.5, 380: 17407.7, 420: 17592.6,
  476: 17728.5, 564: 18090.4, 596: 17917.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 19, 1984, 4.4 ppmC HMW SynAuto (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =           0.254,
NO2    =          0.085,
PAR      =        0.940,
TOL      =        0.228,
XYL      =        0.204,
(NR      =        0.212,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0060,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\st1984.lIx;
TEMPERATURE= (ST 19 84)
    0:  280.3,    60:  280.9,   120:  287.4,
  180:  291.9,   240:  297.2,   300:  298.9,   360:  300.7,
  420:  301.4,   480:  301.9,   540:  301.8,   600:  300.0;
WATER= (RED ST 19 84)
    0: 9500.0,   60: 9500.0,  164: 15744.7, 196: 16801.1,
  236: 17126.1, 308: 17175.5, 380: 17407.7, 420: 17592.6,
  476: 17728.5, 564: 18090.4, 596: 17917.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
September 19, 1984, 2.6 ppmC HMW SynAuto (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =        0.252,
NO2     =        0.086,
ALK7    =        0.072,
TOLU    =        0.140,
XYLE    =        0.088,
TMBZ    =        0.037,
(NROG   =        0.019,
 MISS   =        0.152)
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0060,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST1984.1Ix;
TEMPERATURE= (ST 19 84)
    0:  280.3,    60:  280.9,   120:  287.4,
  180:  291.9,   240:  297.2,   300:  298.9,   360:  300.7,
  420:  301.4,   480:  301.9,   540:  301.8,   600:  300.0;
WATER= (BLUE ST 19 84)
    0: 9500.0,   60: 9500.0,  168: 12408.7,  240: 12350.1,
  312: 12973.4, 360: 13499.8, 424: 13680.0,  480: 13758.0,
  544: 13889.0, 600: 14128.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 19, 1984, 2.6 ppmC HMW SynAuto (BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO   =          0.252,
NO2   =         0.086,
PAR     =       0.571,
TOL     =       0.140,
XYL     =       0.125,
(NR     =       0.138,)
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0060,
CO    =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST1984.lIx;
TEMPERATURE= (ST 19 84)
    0:  280.3,    60:  280.9,   120:  287.4,
  180:  291.9,   240:  297.2,   300:  298.9,   360:  300.7,
  420:  301.4,   480:  301.9,   540:  301.8,   600:  300.0;
WATER= (BLUE ST 19 84)
    0: 9500.0,   60: 9500.0,  168: 12408.7,  240: 12350.1,
  312: 12973.4, 360: 13499.8, 424: 13680.0,  480: 13758.0,
  544: 13889.0, 600: 14128.1;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
September 21, 1984, 2.4 ppmC SynAutoUrb (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =        0.276,
NO2     =        0.087,
ALK4    =        0.055,
ALK7    =        0.032,
ETHE    =        0.301,
PRPE    =        0.050,
TBUT    =        0.014,
TOLU    =        0.066,
XYLE    =        0.046,
TMBZ    =        0.020,
(NROG   =        0.009,
 MISS   =        0.087)
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =          0.0060,
CO      =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST2184.lIx:
TEMPERATURE= (ST 21 84)
    0:  285.5,    60:  286.0,   120:  292.4,
  180:  298.4,   240:  304.5,   300:  305.8,   360:  307.4,
  420:  308.2,   480:  308.4,   540:  307.8,   600:  305.8;
WATER= (RED ST 21 84)
    3: 6542.5,   51: 6609.0,   123: 6689.6,  179: 6709.9,
  251: 6764.2,  299: 6950.2,   363: 7240.5,  419: 7570.8,
  483: 8015.1,  539: 8748.9,   603: 9698.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
September 21, 1984, 2.4 ppmC SynAutoUrb (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =             0.276,
NO2    =            0.087,
PAR      =          0.576,
ETH      =          0.301,
OLE      =          0.050,
TOL      =          0.066,
XYL      =          0.066,
RCHO     =          0.028,
(NR      =          0.068,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0060,
CO     =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\st2184.lIx;
TEMPERATURE= (ST 21 84)
    0:  285.5,    60:  286.0,    120:  292.4,
  180:  298.4,   240:  304.5,    300:  305.8,    360:  307.4,
  420:  308.2,   480:  308.4,    540:  307.8,    600:  305.8;
WATER= (RED ST 21 84)
    3: 6542.5,    51: 6609.0,   123: 6689.6,   179: 6709.9,
  251: 6764.2,   299: 6950.2,   363: 7240.5,   419: 7570.8,
  483: 8015.1,   539: 8748.9,   603: 9698.3;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 21, 1984, 2.4 ppmC SynAutoUrb w/10% HCHO (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =        0.275,
NO2     =        0.085,
ALK4    =        0.055,
ALK7    =        0.033,
ETHE    =        0.298,
PRPE    =        0.052,
TBUT    =        0.014,
TOLU    =        0.066,
XYLE    =        0.046,
TMBZ    =        0.020,
HCHO    =        0.184,
(NROG   =        0.010,
 MISS   =        0.087)
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO    =   0.0038,
ALD2    =   0.0030,
HONO    =           0.0060,
CO      =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\ST2184.1Ix;
TEMPERATURE= (ST 21 84)
    0:  285.5,    60:  286.0,    120:  292.4,
  180:  298.4,   240:  304.5,    300:  305.8,    360:  307.4,
  420:  308.2,   480:  308.4,    540:  307.8,    600:  305.8;
WATER= (BLUE ST 21 84)
    0: 8997.6,   31: 9119.9,   71: 9006.3,  119: 9119.9,
  183: 9137.5,  247: 9208.2,  295: 9333.0,  359: 9615.0,
  423: 10057.3, 479: 10438.6, 543: 11220.9, 599: 12013.8;
.DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=           600;
FINISH
!
```

```
September 21, 1984, 2.4 ppmC SynAutoUrb w/10% HCHO (BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =           0.275,
NO2    =          0.087,
PAR      =        0.576,
ETH      =        0.301,
OLE      =        0.050,
TOL      =        0.066,
XYL      =        0.066,
HCHO     =        0.184,
RCHO     =        0.028,
(NR      =        0.068,)
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0060,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\ST2184.lIx;
TEMPERATURE= (ST 21 84)
    0:  285.5,    60:  286.0,   120:  292.4,
  180:  298.4,   240:  304.5,   300:  305.8,   360:  307.4,
  420:  308.2,   480:  308.4,   540:  307.8,   600:  305.8;
WATER= (BLUE ST 21 84)
    0: 8997.6,   31: 9119.9,   71: 9006.3,  119: 9119.9,
  183: 9137.5,  247: 9208.2,  295: 9333.0,  359: 9615.0,
  423: 10057.3, 479: 10438.6, 543: 11220.9, 599: 12013.8;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 26, 1985 2.27 ppmC SYNURBAN (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO    =              0.264,
NO2    =             0.035,
ETHE     =        0.0783,
PRPE     =        0.0392,
TBUT     =        0.0161,
ALK4     =        0.0896,
ALK7     =        0.1340,
TOLU     =        0.0419,
XYLE     =        0.0251,
TMBZ     =        0.0096,
HCHO     =        0.0400,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO  =.   0.0038,
ALD2  =   0.0030,
HONO  =          0.0024,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=c:\pkss\lix\jn2685.lix;
TEMPERATURE= (June 26, 1985)
   0 : 292.6 ,  60 : 292.6 , 120 : 296.2 , 180 : 300.3 , 240 :
303.8 ,
 300 : 305.7 , 360 : 307.1 , 420 : 308.5 , 480 : 308.0 , 540 :
308.1 ,
 600 : 304.7 ;
WATER= (June 26, 1985, RED)
 -50 : 15529.35 , 420 : 16201.95 , 670 : 15809.6 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
June 26, 1985 2.27 ppmC SYNURBAN (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO   =             0.264,
NO2   =            0.035,
ETH     =       0.0783,
OLE     =       0.0392,
PAR     =       1.3074,
TOL     =       0.0419,
XYL     =       0.0347,
HCHO    =       0.0400,
RCHO    =       0.0252,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0024,
CO    =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=c:\pkss\lix\jn2685.lix;
TEMPERATURE= (June 26, 1985)
   0 : 292.6 ,  60 : 292.6 , 120 : 296.2 , 180 : 300.3 , 240 :
303.8 ,
 300 : 305.7 , 360 : 307.1 , 420 : 308.5 , 480 : 308.0 , 540 :
308.1 ,
 600 : 304.7 ;
WATER= (June 26, 1985, RED)
 -50 : 15529.35 , 420 : 16201.95 , 670 : 15809.6 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 26, 1985 3.1 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO    =              0.266,
NO2    =             0.034,
ETHE     =        0.1100,
PRPE     =        0.0568,
TBUT     =        0.0212,
ALK4     =        0.1242,
ALK7     =        0.1841,
TOLU     =        0.0549,
XYLE     =        0.0319,
TMBZ     =        0.0132,
HCHO     =        0.0597,
        (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =          0.0024,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,TMBZ,
HCHO,ALD2,RCHO,
MEK,MEOH;
EXTR=c:\pkss\lix\jn2685.lix;
TEMPERATURE= (June 26, 1985)
   0 : 292.6 ,  60 : 292.6 , 120 : 296.2 , 180 : 300.3 , 240 :
303.8 ,
 300 : 305.7 , 360 : 307.1 , 420 : 308.5 , 480 : 308.0 , 540 :
308.1 ,
 600 : 304.7 ;
WATER= (June 26, 1985, blue)
 -57 : 16439.2 , 424 : 16862.0 , 658 : 17658.3 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 26, 1985 3.1 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =        0.266,
NO2   =        0.034,
ETH   =        0.1100,
OLE   =        0.0568,
PAR   =        1.8097,
TOL   =        0.0549,
XYL   =        0.0451,
HCHO  =        0.0597,
RCHO  =        0.0329,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0024,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\JN2685.LIX;
TEMPERATURE= (June 26, 1985)
   0 : 292.6 ,  60 : 292.6 , 120 : 296.2 , 180 : 300.3 , 240 :
303.8 ,
 300 : 305.7 , 360 : 307.1 , 420 : 308.5 , 480 : 308.0 , 540 :
308.1 ,
 600 : 304.7 ;
WATER= (June 26, 1985, blue)
 -57 : 16439.2 , 424 : 16862.0 , 658 : 17658.3 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 26, 1985 2.27 ppmC SYNURBAN (RED)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO    =              0.264,
NO2    =             0.035,
ETH      =        0.0783,
OLE      =        0.0553,
ALK      =        0.2236,
AROM     =        0.0900,
HCHO     =        0.0400,
        (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =           0.0024,
CO    =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=c:\pkss\lix\jn2685.lix;
TEMPERATURE= (June 26, 1985)
   0 : 292.6 ,  60 : 292.6 , 120 : 296.2 , 180 : 300.3 , 240 :
303.8 ,
 300 : 305.7 , 360 : 307.1 , 420 : 308.5 , 480 : 308.0 , 540 :
308.1 ,
 600 : 304.7 ;
EMISSIONS=2#
  0: 3.42E-3, 1.17E-5,
 60: 3.42E-3, 1.17E-5,
120: 3.38E-3, 1.14E-5,
180: 3.33E-3, 1.11E-5,
240: 3.29E-3, 1.08E-5,
300: 3.27E-3, 1.07E-5,
360: 3.26E-3, 1.06E-5,
420: 3.25E-3, 1.05E-5,
540: 3.25E-3, 1.05E-5,
600: 3.28E-3, 1.08E-5;
WATER= (June 26, 1985, RED)
 -50 : 15529.35 , 420 : 16201.95 , 670 : 15809.6 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 26, 1985 3.1 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO   =              0.266,
NO2   =             0.034,
ETH     =        0.1100,
OLE     =        0.0780,
ALK     =        0.3083,
AROM    =        0.1179,
HCHO    =        0.0597,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =             0.0024,
CO    =             0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=c:\pkss\lix\jn2685.lix;
TEMPERATURE= (June 26, 1985)
   0 : 292.6 ,  60 : 292.6 , 120 : 296.2 , 180 : 300.3 , 240 :
303.8 ,
 300 : 305.7 , 360 : 307.1 , 420 : 308.5 , 480 : 308.0 , 540 :
308.1 ,
 600 : 304.7 ;
EMISSIONS=2#
  0: 3.42E-3, 1.17E-5,
 60: 3.42E-3, 1.17E-5,
120: 3.38E-3, 1.14E-5,
180: 3.33E-3, 1.11E-5,
240: 3.29E-3, 1.08E-5,
300: 3.27E-3, 1.07E-5,
360: 3.26E-3, 1.06E-5,
420: 3.25E-3, 1.05E-5,
540: 3.25E-3, 1.05E-5,
600: 3.28E-3, 1.08E-5;
WATER= (June 26, 1985, blue)
 -57 : 16439.2 , 424 : 16862.0 , 658 : 17658.3 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 26, 1985 2.27 ppmC SYNURBAN (RED)
C:\PKSS\mech\citchmw2.pks
CONC:
NO   =              0.264,
NO2   =             0.035,
ETH     =        0.0783,
OLE     =        0.0553,
ALK     =        0.2236,
AROM    =        0.0900,
HCHO    =        0.0400,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0024,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=c:\pkss\lix\jn2685.lix;
TEMPERATURE= (June 26, 1985)
   0 : 292.6 ,  60 : 292.6 , 120 : 296.2 , 180 : 300.3 , 240 :
303.8 ,
 300 : 305.7 , 360 : 307.1 , 420 : 308.5 , 480 : 308.0 , 540 :
308.1 ,
 600 : 304.7 ;
EMISSIONS=2#
  0: 3.42E-3, 1.17E-5,
 60: 3.42E-3, 1.17E-5,
120: 3.38E-3, 1.14E-5,
180: 3.33E-3, 1.11E-5,
240: 3.29E-3, 1.08E-5,
300: 3.27E-3, 1.07E-5,
360: 3.26E-3, 1.06E-5,
420: 3.25E-3, 1.05E-5,
540: 3.25E-3, 1.05E-5,
600: 3.28E-3, 1.08E-5;
WATER= (June 26, 1985, RED)
 -50 : 15529.35 , 420 : 16201.95 , 670 : 15809.6 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 26, 1985 3.1 ppmC SYNURBAN (BLUE)
C:\PKSS\mech\citchmw2.pks
CONC:
NO    =              0.266,
NO2    =             0.034,
ETH      =        0.1100,
OLE      =        0.0780,
ALK      =        0.3083,
AROM     =        0.1179,
HCHO     =        0.0597,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =           0.0024,
CO    =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=c:\pkss\lix\jn2685.lix;
TEMPERATURE= (June 26, 1985)
   0 : 292.6 ,  60 : 292.6 , 120 : 296.2 , 180 : 300.3 , 240 :
303.8 ,
 300 : 305.7 , 360 : 307.1 , 420 : 308.5 , 480 : 308.0 , 540 :
308.1 ,
 600 : 304.7 ;
EMISSIONS=2#
  0: 3.42E-3, 1.17E-5,
 60: 3.42E-3, 1.17E-5,
120: 3.38E-3, 1.14E-5,
180: 3.33E-3, 1.11E-5,
240: 3.29E-3, 1.08E-5,
300: 3.27E-3, 1.07E-5,
360: 3.26E-3, 1.06E-5,
420: 3.25E-3, 1.05E-5,
540: 3.25E-3, 1.05E-5,
600: 3.28E-3, 1.08E-5;
WATER= (June 26, 1985, blue)
 -57 : 16439.2 , 424 : 16862.0 , 658 : 17658.3 ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
JUNE 28, 1985 1.24 ppmC SYNURBAN (RED)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO      =        0.273,
NO2     =        0.107,
ETHE    =        0.0718,
PRPE    =        0.0353,
TBUT    =        0.0139,
ALK4    =        0.1390,
ALK7    =        0.1324,
TOLU    =        0.0386,
XYLE    =        0.0221,
TMBZ    =        0.0108,
HCHO    =        0.0390,
       (Surface NMHC = 0.0380 ppmC)
ALK4    =   0.0201,
ETHE    =   0.0009,
PRPE    =   0.0006,
TOLU    =   0.0004,
XYLE    =   0.0003,
HCHO   =   0.0038,
ALD2   =   0.0030,
HONO   =          0.0075,
CO     =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\JN2885.LIX;
TEMPERATURE=  (JUNE 28 1985)
   6 : 284.3 ,  66 : 284.9 , 126 : 289.5 , 186 : 297.1 , 246 :
300.2 ,
 306 : 302.9 , 365 : 304.4 , 426 : 305.2 , 486 : 303.7 , 546 :
304.9 ,
 606 : 307.3 ;
WATER=     (JUNE 28 1985, RED)
 -42 : 6200. ,  398 : 7000. , 641 : 7800. ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=         600;
FINISH
!
```

```
JUNE 28, 1985 2.39 ppmC SYNURBAN (RED)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO    =       0.273,
NO2   =       0.107,
ETH   =       0.0718,
OLE   =       0.0353,
PAR   =       1.5001,
TOL   =       0.0386,
XYL   =       0.0329,
HCHO  =       0.0390,
RCHO  =       0.0213,
PAR   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
TOL   =   0.0004,
XYL   =   0.0003,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =   0.0075,
CO    =         0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\JN2885.LIX;
TEMPERATURE=  (JUNE 28 1985)
   6 : 284.3 ,  66 : 284.9 , 126 : 289.5 , 186 : 297.1 , 246 :
300.2 ,
 306 : 302.9 , 365 : 304.4 , 426 : 305.2 , 486 : 303.7 , 546 :
304.9 ,
 606 : 307.3 ;
WATER=     (JUNE 28 1985, RED)
 -42 : 6200. ,  398 : 7000. , 641 : 7800. ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
JUNE 28, 1985 1.24 ppmC SYNURBAN (RED)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO      =         0.273,
NO2     =         0.107,
ETH     =         0.0718,
OLE     =         0.0492,
ALK     =         0.2714,
AROM    =         0.0832,
HCHO    =         0.0390,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =            0.0075,
CO    =            0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\JN2885.LIX;
TEMPERATURE=  (JUNE 28 1985)
   6 : 284.3 ,  66 : 284.9 , 126 : 289.5 , 186 : 297.1 , 246 :
300.2 ,
 306 : 302.9 , 365 : 304.4 , 426 : 305.2 , 486 : 303.7 , 546 :
304.9 ,
 606 : 307.3 ;
EMISSIONS=2#
  6: 3.52E-3, 1.24E-5,
 66: 3.51E-3, 1.23E-5,
126: 3.45E-3, 1.19E-5,
186: 3.37E-3, 1.13E-5,
246: 3.33E-3, 1.11E-5,
306: 3.30E-3, 1.09E-5,
365: 3.28E-3, 1.08E-5,
426: 3.28E-3, 1.07E-5,
486: 3.29E-3, 1.08E-5,
546: 3.28E-3, 1.08E-5,
606: 3.25E-3, 1.06E-5;
WATER=     (JUNE 28 1985, RED)
 -42 : 6200. ,  398 : 7000. , 641 : 7800. ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
JUNE 28, 1985 1.24 ppmC SYNURBAN (RED)
C:\PKSS\mech\citchmw2.pks
CONC:
NO      =        0.273,
NO2     =        0.107,
ETH     =        0.0718,
OLE     =        0.0492,
ALK     =        0.2714,
AROM    =        0.0832,
HCHO    =        0.0390,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0075,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\JN2885.LIX;
TEMPERATURE=  (JUNE 28 1985)
   6 : 284.3 ,  66 : 284.9 , 126 : 289.5 , 186 : 297.1 , 246 :
300.2 ,
 306 : 302.9 , 365 : 304.4 , 426 : 305.2 , 486 : 303.7 , 546 :
304.9 ,
 606 : 307.3 ;
EMISSIONS=2#
  6: 3.52E-3, 1.24E-5,
 66: 3.51E-3, 1.23E-5,
126: 3.45E-3, 1.19E-5,
186: 3.37E-3, 1.13E-5,
246: 3.33E-3, 1.11E-5,
306: 3.30E-3, 1.09E-5,
365: 3.28E-3, 1.08E-5,
426: 3.28E-3, 1.07E-5,
486: 3.29E-3, 1.08E-5,
546: 3.28E-3, 1.08E-5,
606: 3.25E-3, 1.06E-5;
WATER=     (JUNE 28 1985, RED)
 -42 : 6200. ,  398 : 7000. , 641 : 7800. ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 28, 1985 1.32 ppmC SYNURBAN, 0.58 ppm MeOH, 0.7 ppm HCHO
(BLUE)
C:\PKSS\mech\CALCHMW.pks
CONC:
NO   =              0.275,
NO2   =             0.112,
ETHE     =       0.0452,
PRPE     =       0.0203,
TBUT     =       0.0082,
ALK4     =       0.0457,
ALK7     =       0.0798,
TOLU     =       0.0253,
XYLE     =       0.0146,
TMBZ     =       0.0072,
HCHO     =       0.0908,
MEOH     =       0.5823,
       (Surface NMHC = 0.0380 ppmC)
ALK4   =   0.0201,
ETHE   =   0.0009,
PRPE   =   0.0006,
TOLU   =   0.0004,
XYLE   =   0.0003,
HCHO  =   0.0038,
ALD2  =   0.0030,
HONO  =          0.0078,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK4,ALK7,ETHE,PRPE,TBUT,TOLU,XYLE,
TMBZ,HCHO,ALD2,RCHO,MEK,MEOH;
EXTR=C:\PKSS\LIX\JN2885.LIX;
TEMPERATURE=  (JUNE 28 1985)
   6 : 284.3 ,  66 : 284.9 , 126 : 289.5 , 186 : 297.1 , 246 :
300.2 ,
 306 : 302.9 , 365 : 304.4 , 426 : 305.2 , 486 : 303.7 , 546 :
304.9 ,
 606 : 307.3 ;
WATER=     (JUNE 28 1985, BLUE)
 -46 : 11051.75 ,  394 : 12135. , 645 : 12135. ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 28, 1985 1.32 ppmC SYNURBAN, 0.58 ppm MeOH, 0.07 ppm HCHO
(BLUE)
C:\PKSS\mech\cb42CHMW.pks
CONC:
NO   =              0.275,
NO2   =             0.112,
ETH      =       0.0452,
OLE      =       0.0203,
PAR      =       0.7539,
TOL      =       0.0253,
XYL      =       0.0218,
HCHO     =       0.0908,
MEOH     =       0.5823,
RCHO     =       0.0125,
PAR    =   0.0201,
ETH    =   0.0009,
OLE    =   0.0006,
TOL    =   0.0004,
XYL    =   0.0003,
HCHO   =   0.0038,
RCHO   =   0.0030,
HONO   =   0.0078,
CO     =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,PAR,ETH,OLE,TOL,XYL,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\JN2885.LIX;
TEMPERATURE=  (JUNE 28 1985)
   6 : 284.3 ,  66 : 284.9 , 126 : 289.5 , 186 : 297.1 , 246 :
300.2 ,
 306 : 302.9 , 365 : 304.4 , 426 : 305.2 , 486 : 303.7 , 546 :
304.9 ,
 606 : 307.3 ;
WATER=      (JUNE 28 1985, BLUE)
 -46 : 11051.75 ,  394 : 12135. , 645 : 12135. ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 28, 1985 1.32 ppmC SYNURBAN, 0.58 ppm MeOH, 0.7 ppm HCHO
(BLUE)
C:\PKSS\mech\CITCHMW.pks
CONC:
NO    =              0.275,
NO2   =              0.112,
ETH      =        0.0452,
OLE      =        0.0766,
ALK      =        0.1255,
AROM     =        0.0548,
HCHO     =        0.0908,
MEOH     =        0.5823,
        (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =           0.0078,
CO    =           0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\JN2885.LIX;
TEMPERATURE=  (JUNE 28 1985)
   6 : 284.3 ,  66 : 284.9 , 126 : 289.5 , 186 : 297.1 , 246 :
300.2 ,
 306 : 302.9 , 365 : 304.4 , 426 : 305.2 , 486 : 303.7 , 546 :
304.9 ,
 606 : 307.3 ;
EMISSIONS=2#
  6: 3.52E-3, 1.24E-5,
 66: 3.51E-3, 1.23E-5,
126: 3.45E-3, 1.19E-5,
186: 3.37E-3, 1.13E-5,
246: 3.33E-3, 1.11E-5,
306: 3.30E-3, 1.09E-5,
365: 3.28E-3, 1.08E-5,
426: 3.28E-3, 1.07E-5,
486: 3.29E-3, 1.08E-5,
546: 3.28E-3, 1.08E-5,
606: 3.25E-3, 1.06E-5;
WATER=     (JUNE 28 1985, BLUE)
 -46 : 11051.75 ,  394 : 12135. , 645 : 12135. ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

```
June 28, 1985 1.32 ppmC SYNURBAN, 0.58 ppm MeOH, 0.7 ppm HCHO
(BLUE)
C:\PKSS\mech\citchmw2.pks
CONC:
NO   =              0.275,
NO2   =             0.112,
ETH      =       0.0452,
OLE      =       0.0766,
ALK      =       0.1255,
AROM     =       0.0548,
HCHO     =       0.0908,
MEOH     =       0.5823,
       (Surface NMHC = 0.0380 ppmC)
ALK   =   0.0201,
ETH   =   0.0009,
OLE   =   0.0006,
AROM  =   0.0007,
HCHO  =   0.0038,
RCHO  =   0.0030,
HONO  =          0.0078,
CO    =          0.3;
PRINT=
O3,NO,NO2,HNO3,PAN,CO,ALK,ETH,OLE,AROM,HCHO,RCHO,MEOH;
EXTR=C:\PKSS\LIX\JN2885.LIX;
TEMPERATURE=  (JUNE 28 1985)
   6 : 284.3 ,  66 : 284.9 , 126 : 289.5 , 186 : 297.1 , 246 :
300.2 ,
 306 : 302.9 , 365 : 304.4 , 426 : 305.2 , 486 : 303.7 , 546 :
304.9 ,
 606 : 307.3 ;
EMISSIONS=2#
  6: 3.52E-3, 1.24E-5,
 66: 3.51E-3, 1.23E-5,
126: 3.45E-3, 1.19E-5,
186: 3.37E-3, 1.13E-5,
246: 3.33E-3, 1.11E-5,
306: 3.30E-3, 1.09E-5,
365: 3.28E-3, 1.08E-5,
426: 3.28E-3, 1.07E-5,
486: 3.29E-3, 1.08E-5,
546: 3.28E-3, 1.08E-5,
606: 3.25E-3, 1.06E-5;
WATER=     (JUNE 28 1985, BLUE)
 -46 : 11051.75 ,  394 : 12135. , 645 : 12135. ;
DILUTION=
  0: 1.5E-4, 610: 1.5E-4;
CONT=
TMAX=          600;
FINISH
!
```

Appendix C

Photolytic Rate Tables for Model Simulations

This appendix contains all of the actual photolytic rate tables used by PKSS-PC to generate the plots in Appendix A. There is one rate table for each day. The columns in the table correspond to the /Lx designations in the mechanism listings provided in the body of this report. The number x refers to the column in these tables.

August 4, 1984

```
("NO2")
("HCHOr")
("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
LIGHT=6#
   0 (0627): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
   9 (0636): 0.0014, 0.0008, 0.0026, 0.0001, 0.0001,  3.1434,
  25 (0652): 0.0113, 0.0082, 0.0244, 0.0003, 0.0005,  3.6934,
  41 (0708): 0.0214, 0.0193, 0.0486, 0.0014, 0.0014,  5.2929,
  57 (0724): 0.0371, 0.0331, 0.0759, 0.0044, 0.0028,  7.6235,
  73 (0740): 0.0657, 0.0608, 0.1324, 0.0120, 0.0058, 10.7431,
  89 (0756): 0.1049, 0.1054, 0.2191, 0.0283, 0.0110, 14.2926,
 105 (0812): 0.1517, 0.1682, 0.3338, 0.0576, 0.0189, 18.0039,
 121 (0828): 0.2008, 0.2452, 0.4655, 0.1030, 0.0294, 21.4688,
 137 (0844): 0.2514, 0.3363, 0.6124, 0.1682, 0.0428, 24.7647,
 153 (0900): 0.2990, 0.4319, 0.7571, 0.2512, 0.0580, 28.1049,
 169 (0916): 0.3472, 0.5395, 0.9138, 0.3572, 0.0760, 30.9965,
 185 (0932): 0.3925, 0.6499, 1.0679, 0.4814, 0.0955, 33.6360,
 201 (0948): 0.4347, 0.7606, 1.2166, 0.6205, 0.1160, 36.0542,
 217 (1004): 0.4718, 0.8652, 1.3519, 0.7670, 0.1363, 38.1915,
 233 (1020): 0.5051, 0.9631, 1.4749, 0.9167, 0.1561, 40.1460,
 249 (1036): 0.5360, 1.0571, 1.5907, 1.0696, 0.1755, 41.9939,
 265 (1052): 0.5608, 1.1367, 1.6850, 1.2117, 0.1928, 43.5504,
 281 (1108): 0.5747, 1.1934, 1.7462, 1.3298, 0.2061, 44.2293,
 297 (1124): 0.5849, 1.2387, 1.7927, 1.4330, 0.2172, 44.7246,
 313 (1140): 0.5904, 1.2731, 1.8250, 1.5198, 0.2262, 44.8088,
 329 (1156): 0.6023, 1.3204, 1.8770, 1.6183, 0.2372, 45.3320,
 345 (1212): 0.6125, 1.3603, 1.9208, 1.7029, 0.2465, 45.8469,
 361 (1228): 0.6209, 1.3923, 1.9559, 1.7718, 0.2541, 46.3066,
 377 (1244): 0.6271, 1.4160, 1.9818, 1.8236, 0.2597, 46.6762,
 393 (1300): 0.6311, 1.4312, 1.9983, 1.8573, 0.2634, 46.9290,
 409 (1316): 0.5144, 1.2085, 1.6855, 1.5739, 0.2227, 33.3205,
 425 (1332): 0.5137, 1.2065, 1.6830, 1.5707, 0.2223, 33.2956,
 441 (1348): 0.5111, 1.1972, 1.6724, 1.5517, 0.2202, 33.1576,
 457 (1404): 0.5941, 1.3529, 1.8948, 1.7384, 0.2479, 42.5962,
 473 (1420): 0.5863, 1.3257, 1.8641, 1.6817, 0.2416, 42.1282,
 489 (1436): 0.5763, 1.2904, 1.8242, 1.6090, 0.2335, 41.5240,
 505 (1452): 0.5640, 1.2474, 1.7753, 1.5214, 0.2236, 40.7957,
 521 (1508): 0.5495, 1.1969, 1.7176, 1.4205, 0.2121, 39.9573,
 537 (1524): 0.5307, 1.1332, 1.6430, 1.3012, 0.1981, 38.9216,
 553 (1540): 0.5116, 1.0677, 1.5665, 1.1787, 0.1837, 37.9045,
 569 (1556): 0.4921, 0.9997, 1.4873, 1.0539, 0.1687, 36.9264,
 585 (1612): 0.4282, 0.8489, 1.2836, 0.8476, 0.1402, 31.6898,
 601 (1628): 0.4116, 0.7861, 1.2111, 0.7368, 0.1266, 31.0803,
 617 (1644): 0.3869, 0.7102, 1.1170, 0.6185, 0.1111, 29.7297,
 633 (1700): 0.3582, 0.6275, 1.0105, 0.5018, 0.0950, 28.1603,
 649 (1716): 0.3254, 0.5400, 0.8934, 0.3911, 0.0787, 26.3685,
 665 (1732): 0.2890, 0.4504, 0.7683, 0.2908, 0.0629, 24.3495,
 681 (1748): 0.2488, 0.3606, 0.6367, 0.2037, 0.0480, 22.0603,
 697 (1804): 0.2057, 0.2745, 0.5038, 0.1328, 0.0346, 19.5003,
 713 (1820): 0.1637, 0.1995, 0.3819, 0.0806, 0.0236, 16.8673,
 729 (1836): 0.1220, 0.1350, 0.2701, 0.0441, 0.0149, 14.0165,
 745 (1852): 0.0825, 0.0829, 0.1739, 0.0210, 0.0085, 10.9825;
ENDX;
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August 5, 1984

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("NO2")
("HCHOr")
("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
LIGHT=6#
   0 (0628): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
   8 (0636): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0895,
  24 (0652): 0.0005, 0.0002, 0.0008, 0.0001, 0.0001,  0.5746,
  40 (0708): 0.0039, 0.0027, 0.0072, 0.0002, 0.0002,  1.9054,
  56 (0724): 0.0129, 0.0095, 0.0228, 0.0012, 0.0008,  4.0760,
  72 (0740): 0.0324, 0.0263, 0.0592, 0.0049, 0.0024,  7.1014,
  88 (0756): 0.0634, 0.0585, 0.1245, 0.0149, 0.0060, 10.6873,
 104 (0812): 0.1043, 0.1093, 0.2204, 0.0360, 0.0121, 14.5465,
 120 (0828): 0.1506, 0.1770, 0.3396, 0.0724, 0.0210, 18.3073,
 136 (0844): 0.2000, 0.2604, 0.4774, 0.1280, 0.0329, 21.9190,
 152 (0900): 0.2338, 0.3345, 0.5890, 0.1924, 0.0448, 23.2510,
 168 (0916): 0.2807, 0.4338, 0.7371, 0.2853, 0.0610, 26.2088,
 184 (0932): 0.3257, 0.5380, 0.8857, 0.3970, 0.0790, 28.9420,
 200 (0948): 0.3682, 0.6441, 1.0316, 0.5247, 0.0982, 31.4692,
 216 (1004): 0.4065, 0.7464, 1.1671, 0.6617, 0.1176, 33.7337,
 232 (1020): 0.4407, 0.8427, 1.2907, 0.8032, 0.1366, 35.7810,
 248 (1036): 0.4728, 0.9360, 1.4081, 0.9493, 0.1556, 37.7182,
 264 (1052): 0.4998, 1.0178, 1.5080, 1.0884, 0.1728, 39.4197,
 280 (1108): 0.5163, 1.0777, 1.5757, 1.2053, 0.1864, 40.2862,
 296 (1124): 0.5282, 1.1255, 1.6272, 1.3075, 0.1977, 40.8523,
 312 (1140): 0.5351, 1.1612, 1.6627, 1.3926, 0.2067, 41.0234,
 328 (1156): 0.5474, 1.2087, 1.7159, 1.4886, 0.2176, 41.5726,
 344 (1212): 0.5582, 1.2492, 1.7613, 1.5718, 0.2269, 42.1142,
 360 (1228): 0.5671, 1.2821, 1.7982, 1.6403, 0.2345, 42.6000,
 376 (1244): 0.5740, 1.3070, 1.8260, 1.6924, 0.2403, 42.9942,
 392 (1300): 0.5785, 1.3234, 1.8444, 1.7271, 0.2441, 43.2692,
 408 (1316): 0.5552, 1.2851, 1.7891, 1.6831, 0.2374, 39.8742,
 424 (1332): 0.5545, 1.2829, 1.7863, 1.6793, 0.2370, 39.8438,
 440 (1348): 0.5514, 1.2723, 1.7741, 1.6579, 0.2346, 39.6655,
 456 (1404): 0.5459, 1.2534, 1.7525, 1.6192, 0.2302, 39.3373,
 472 (1420): 0.5380, 1.2265, 1.7216, 1.5640, 0.2241, 38.8623,
 488 (1436): 0.5278, 1.1916, 1.6817, 1.4933, 0.2161, 38.2484,
 504 (1452): 0.5153, 1.1492, 1.6328, 1.4085, 0.2065, 37.5084,
 520 (1508): 0.5058, 1.0989, 1.5745, 1.3104, 0.1952, 38.6791,
 536 (1524): 0.4871, 1.0374, 1.5018, 1.1964, 0.1817, 37.6031,
 552 (1540): 0.4680, 0.9737, 1.4267, 1.0793, 0.1678, 36.5299,
 568 (1556): 0.4483, 0.9077, 1.3487, 0.9603, 0.1535, 35.4872,
 584 (1612): 0.4287, 0.8402, 1.2691, 0.8414, 0.1389, 34.5547,
 600 (1628): 0.4083, 0.7702, 1.1857, 0.7233, 0.1241, 33.6868,
 616 (1644): 0.3786, 0.6858, 1.0782, 0.5977, 0.1073, 31.9022,
 632 (1700): 0.3446, 0.5951, 0.9584, 0.4753, 0.0900, 29.8595,
 648 (1716): 0.3067, 0.5005, 0.8288, 0.3611, 0.0728, 27.5574,
 664 (1732): 0.2652, 0.4051, 0.6925, 0.2596, 0.0564, 24.9948,
 680 (1748): 0.2206, 0.3116, 0.5525, 0.1739, 0.0413, 22.1421,
 696 (1804): 0.1790, 0.2363, 0.4365, 0.1120, 0.0295, 17.9239,
 712 (1820): 0.1331, 0.1582, 0.3062, 0.0620, 0.0185, 14.8574,
 728 (1836): 0.0896, 0.0946, 0.1927, 0.0296, 0.0103, 11.6073,
 744 (1852): 0.0520, 0.0482, 0.1037, 0.0115, 0.0048,  8.2931;
ENDX;
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August 6, 1984

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("HCHOr")
("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
LIGHT=6#
   0 (0629): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
  11 (0640): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0019,
  27 (0656): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0682,
  43 (0712): 0.0012, 0.0007, 0.0019, 0.0001, 0.0001,  0.7688,
  59 (0728): 0.0077, 0.0052, 0.0125, 0.0007, 0.0004,  2.7468,
  75 (0744): 0.0254, 0.0197, 0.0444, 0.0040, 0.0019,  5.8491,
  91 (0800): 0.0564, 0.0508, 0.1080, 0.0137, 0.0053,  9.7047,
 107 (0816): 0.0994, 0.1029, 0.2070, 0.0356, 0.0115, 13.8974,
 123 (0832): 0.1489, 0.1746, 0.3339, 0.0742, 0.0210, 17.9486,
 139 (0848): 0.2022, 0.2645, 0.4829, 0.1342, 0.0338, 21.8050,
 155 (0904): 0.2438, 0.3513, 0.6156, 0.2076, 0.0474, 23.9357,
 171 (0920): 0.2931, 0.4576, 0.7735, 0.3082, 0.0649, 26.9875,
 187 (0936): 0.3402, 0.5686, 0.9314, 0.4285, 0.0841, 29.7718,
 203 (0952): 0.3856, 0.6832, 1.0886, 0.5669, 0.1049, 32.4125,
 219 (1008): 0.4247, 0.7890, 1.2281, 0.7108, 0.1251, 34.6964,
 235 (1024): 0.4596, 0.8880, 1.3547, 0.8580, 0.1448, 36.7623,
 251 (1040): 0.4922, 0.9838, 1.4748, 1.0094, 0.1643, 38.7241,
 267 (1056): 0.5184, 1.0639, 1.5718, 1.1488, 0.1814, 40.3876,
 283 (1112): 0.5338, 1.1222, 1.6369, 1.2655, 0.1947, 41.1249,
 299 (1128): 0.5436, 1.1669, 1.6833, 1.3648, 0.2056, 41.4800,
 315 (1144): 0.5520, 1.2064, 1.7240, 1.4548, 0.2152, 41.7544,
 331 (1200): 0.5645, 1.2539, 1.7774, 1.5510, 0.2261, 42.3216,
 347 (1216): 0.5752, 1.2941, 1.8224, 1.6335, 0.2354, 42.8663,
 363 (1232): 0.5840, 1.3263, 1.8586, 1.7004, 0.2428, 43.3439,
 379 (1248): 0.5905, 1.3501, 1.8853, 1.7501, 0.2484, 43.7203,
 395 (1304): 0.5935, 1.3700, 1.9090, 1.7880, 0.2527, 42.8954,
 411 (1320): 0.5946, 1.3741, 1.9133, 1.7979, 0.2538, 42.9749,
 427 (1336): 0.5932, 1.3693, 1.9076, 1.7888, 0.2527, 42.9005,
 443 (1352): 0.5891, 1.3556, 1.8918, 1.7609, 0.2496, 42.6654,
 459 (1408): 0.5825, 1.3330, 1.8660, 1.7147, 0.2444, 42.2691,
 475 (1424): 0.5734, 1.3018, 1.8303, 1.6511, 0.2373, 41.7161,
 491 (1440): 0.5618, 1.2623, 1.7849, 1.5712, 0.2283, 41.0163,
 507 (1456): 0.5478, 1.2148, 1.7301, 1.4767, 0.2175, 40.1846,
 523 (1512): 0.5299, 1.1485, 1.6503, 1.3560, 0.2032, 40.1292,
 539 (1528): 0.5099, 1.0824, 1.5723, 1.2340, 0.1887, 38.9990,
 555 (1544): 0.4894, 1.0140, 1.4916, 1.1089, 0.1738, 37.8773,
 571 (1600): 0.4684, 0.9430, 1.4077, 0.9821, 0.1584, 36.7970,
 587 (1616): 0.4475, 0.8704, 1.3219, 0.8556, 0.1429, 35.8563,
 603 (1632): 0.4231, 0.7913, 1.2256, 0.7273, 0.1264, 34.6892,
 619 (1648): 0.3901, 0.6990, 1.1067, 0.5941, 0.1083, 32.7321,
 635 (1704): 0.3526, 0.6007, 0.9754, 0.4660, 0.0899, 30.5040,
 651 (1720): 0.3111, 0.4994, 0.8348, 0.3482, 0.0718, 28.0040,
 667 (1736): 0.2661, 0.3985, 0.6885, 0.2454, 0.0547, 25.2324,
 683 (1752): 0.2184, 0.3011, 0.5405, 0.1603, 0.0392, 22.1875,
 699 (1808): 0.1655, 0.2117, 0.3966, 0.0951, 0.0260, 17.0533,
 715 (1824): 0.1201, 0.1379, 0.2709, 0.0507, 0.0158, 13.9277,
 731 (1840): 0.0776, 0.0788, 0.1632, 0.0229, 0.0084, 10.6071,
 747 (1856): 0.0428, 0.0381, 0.0835, 0.0083, 0.0037,  7.3573;
ENDX;
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August 7, 1984

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("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
LIGHT=6#
   0 (0630): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
  10 (0640): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0559,
  26 (0656): 0.0005, 0.0002, 0.0008, 0.0001, 0.0001,  0.5680,
  42 (0712): 0.0040, 0.0027, 0.0071, 0.0002, 0.0002,  2.0181,
  58 (0728): 0.0141, 0.0102, 0.0243, 0.0014, 0.0009,  4.4637,
  74 (0744): 0.0358, 0.0289, 0.0646, 0.0057, 0.0027,  7.8467,
  90 (0800): 0.0697, 0.0644, 0.1361, 0.0172, 0.0066, 11.8176,
 106 (0816): 0.1138, 0.1198, 0.2397, 0.0410, 0.0134, 16.0399,
 122 (0832): 0.1628, 0.1924, 0.3665, 0.0813, 0.0231, 20.0866,
 138 (0848): 0.2151, 0.2816, 0.5129, 0.1424, 0.0360, 23.9567,
 154 (0904): 0.2499, 0.3632, 0.6356, 0.2140, 0.0490, 24.2998,
 170 (0920): 0.2985, 0.4681, 0.7908, 0.3144, 0.0663, 27.3116,
 186 (0936): 0.3449, 0.5774, 0.9458, 0.4338, 0.0853, 30.0920,
 202 (0952): 0.3885, 0.6879, 1.0969, 0.5691, 0.1055, 32.6560,
 218 (1008): 0.4266, 0.7910, 1.2324, 0.7104, 0.1253, 34.9023,
 234 (1024): 0.4607, 0.8878, 1.3560, 0.8552, 0.1445, 36.9478,
 250 (1040): 0.4927, 0.9815, 1.4732, 1.0039, 0.1637, 38.8932,
 266 (1056): 0.5186, 1.0601, 1.5685, 1.1411, 0.1805, 40.5543,
 282 (1112): 0.5337, 1.1170, 1.6318, 1.2555, 0.1935, 41.3200,
 298 (1128): 0.5424, 1.1589, 1.6745, 1.3508, 0.2038, 41.5828,
 314 (1144): 0.5498, 1.1953, 1.7111, 1.4362, 0.2129, 41.8185,
 330 (1200): 0.5617, 1.2410, 1.7623, 1.5294, 0.2234, 42.3744,
 346 (1216): 0.5627, 1.2643, 1.7840, 1.5898, 0.2296, 41.4344,
 362 (1232): 0.5709, 1.2944, 1.8177, 1.6530, 0.2366, 41.8843,
 378 (1248): 0.5769, 1.3163, 1.8420, 1.6993, 0.2417, 42.2354,
 394 (1304): 0.5806, 1.3296, 1.8568, 1.7280, 0.2448, 42.4629,
 410 (1320): 0.5819, 1.3343, 1.8619, 1.7385, 0.2459, 42.5497,
 426 (1336): 0.5806, 1.3301, 1.8570, 1.7304, 0.2450, 42.4816,
 442 (1352): 0.5768, 1.3171, 1.8421, 1.7039, 0.2420, 42.2524,
 458 (1408): 0.5703, 1.2953, 1.8171, 1.6593, 0.2370, 41.8613,
 474 (1424): 0.5614, 1.2651, 1.7824, 1.5976, 0.2301, 41.3130,
 490 (1440): 0.5500, 1.2265, 1.7380, 1.5200, 0.2214, 40.6173,
 506 (1456): 0.5362, 1.1800, 1.6843, 1.4280, 0.2109, 39.7888,
 522 (1512): 0.5207, 1.1221, 1.6162, 1.3188, 0.1981, 39.5276,
 538 (1528): 0.5008, 1.0570, 1.5390, 1.1991, 0.1839, 38.4016,
 554 (1544): 0.4804, 0.9893, 1.4588, 1.0764, 0.1692, 37.2814,
 570 (1600): 0.4595, 0.9195, 1.3760, 0.9524, 0.1541, 36.2068,
 586 (1616): 0.4385, 0.8475, 1.2905, 0.8283, 0.1388, 35.2581,
 602 (1632): 0.4140, 0.7690, 1.1944, 0.7024, 0.1225, 34.0688,
 618 (1648): 0.3811, 0.6780, 1.0765, 0.5723, 0.1048, 32.1190,
 634 (1704): 0.3439, 0.5812, 0.9466, 0.4474, 0.0867, 29.8973,
 650 (1720): 0.3026, 0.4815, 0.8076, 0.3330, 0.0690, 27.4030,
 666 (1736): 0.2579, 0.3825, 0.6633, 0.2334, 0.0523, 24.6370,
 682 (1752): 0.2103, 0.2869, 0.5169, 0.1512, 0.0372, 21.5564,
 698 (1808): 0.1584, 0.1999, 0.3761, 0.0887, 0.0244, 16.6015,
 714 (1824): 0.1139, 0.1288, 0.2543, 0.0467, 0.0147, 13.4813,
 730 (1840): 0.0725, 0.0724, 0.1507, 0.0207, 0.0076, 10.1694,
 746 (1856): 0.0392, 0.0343, 0.0755, 0.0073, 0.0033,  6.9608;
ENDX;
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August 8, 1984

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("NO2")
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("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
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   9 (0640): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
  25 (0656): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0016,
  41 (0712): 0.0008, 0.0005, 0.0012, 0.0001, 0.0001,  0.0692,
  57 (0728): 0.0057, 0.0037, 0.0089, 0.0005, 0.0001,  0.6730,
  73 (0744): 0.0201, 0.0150, 0.0342, 0.0029, 0.0003,  2.3504,
  89 (0800): 0.0471, 0.0414, 0.0886, 0.0108, 0.0014,  5.1591,
 105 (0816): 0.0859, 0.0877, 0.1772, 0.0295, 0.0042,  8.7871,
 121 (0832): 0.1319, 0.1532, 0.2937, 0.0640, 0.0097, 12.8402,
 137 (0848): 0.1824, 0.2367, 0.4329, 0.1187, 0.0183, 16.8466,
 153 (0904): 0.2107, 0.3045, 0.5341, 0.1785, 0.0301, 20.7241,
 169 (0920): 0.2564, 0.4015, 0.6791, 0.2690, 0.0410, 20.9595,
 185 (0936): 0.3016, 0.5055, 0.8284, 0.3796, 0.0568, 23.8225,
 201 (0952): 0.3443, 0.6116, 0.9749, 0.5064, 0.0747, 26.5560,
 217 (1008): 0.3813, 0.7103, 1.1059, 0.6390, 0.0938, 29.0775,
 233 (1024): 0.4142, 0.8022, 1.2241, 0.7744, 0.1126, 31.2713,
 249 (1040): 0.4451, 0.8914, 1.3366, 0.9143, 0.1307, 33.2423,
 265 (1056): 0.4708, 0.9681, 1.4306, 1.0452, 0.1488, 35.1197,
 281 (1112): 0.4866, 1.0243, 1.4945, 1.1551, 0.1650, 36.7644,
 297 (1128): 0.4950, 1.0646, 1.5361, 1.2455, 0.1777, 37.5967,
 313 (1144): 0.5024, 1.0993, 1.5715, 1.3260, 0.1876, 37.8245,
 329 (1200): 0.5140, 1.1434, 1.6212, 1.4146, 0.1961, 38.0710,
 345 (1216): 0.5242, 1.1806, 1.6632, 1.4906, 0.2062, 38.6107,
 361 (1232): 0.5324, 1.2104, 1.6969, 1.5521, 0.2148, 39.1293,
 377 (1248): 0.5386, 1.2324, 1.7216, 1.5977, 0.2216, 39.5840,
 393 (1304): 0.4769, 1.0988, 1.5318, 1.4341, 0.2267, 39.9419,
 409 (1320): 0.4778, 1.1020, 1.5351, 1.4417, 0.2027, 34.8902,
 425 (1336): 0.4764, 1.0977, 1.5300, 1.4337, 0.2035, 34.9538,
 441 (1352): 0.4729, 1.0859, 1.5163, 1.4102, 0.2026, 34.8859,
 457 (1408): 0.4672, 1.0668, 1.4942, 1.3716, 0.1999, 34.6810,
 473 (1424): 0.4594, 1.0405, 1.4639, 1.3187, 0.1956, 34.3382,
 489 (1440): 0.4495, 1.0073, 1.4254, 1.2526, 0.1896, 33.8617,
 505 (1456): 0.4375, 0.9675, 1.3791, 1.1746, 0.1821, 33.2598,
 521 (1512): 0.4662, 1.0092, 1.4519, 1.1896, 0.1731, 32.5451,
 537 (1528): 0.4476, 0.9487, 1.3798, 1.0791, 0.1784, 35.4826,
 553 (1544): 0.4284, 0.8858, 1.3050, 0.9660, 0.1652, 34.4286,
 569 (1600): 0.4090, 0.8214, 1.2281, 0.8524, 0.1516, 33.3745,
 585 (1616): 0.3885, 0.7530, 1.1460, 0.7370, 0.1378, 32.3654,
 601 (1632): 0.3644, 0.6786, 1.0536, 0.6202, 0.1234, 31.4195,
 617 (1648): 0.3329, 0.5931, 0.9418, 0.5005, 0.1082, 30.2262,
 633 (1704): 0.2975, 0.5032, 0.8198, 0.3868, 0.0916, 28.3330,
 649 (1720): 0.2587, 0.4115, 0.6908, 0.2837, 0.0750, 26.1933,
 665 (1736): 0.2174, 0.3217, 0.5587, 0.1953, 0.0589, 23.8101,
 681 (1752): 0.1749, 0.2374, 0.4288, 0.1241, 0.0439, 21.2201,
 697 (1808): 0.1340, 0.1670, 0.3154, 0.0732, 0.0307, 18.3895,
 713 (1824): 0.0931, 0.1033, 0.2052, 0.0368, 0.0203, 14.7171,
 729 (1840): 0.0563, 0.0547, 0.1148, 0.0152, 0.0117, 11.6781,
 745 (1856): 0.0282, 0.0236, 0.0527, 0.0049, 0.0057,  8.5226,
ENDX;                                       0.0023,  5.5563,
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August 9, 1984

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("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
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   9 (0640): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0004,
  25 (0656): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0213,
  41 (0712): 0.0004, 0.0002, 0.0007, 0.0001, 0.0001,  0.3645,
  57 (0728): 0.0038, 0.0024, 0.0059, 0.0003, 0.0002,  1.6277,
  73 (0744): 0.0155, 0.0115, 0.0263, 0.0022, 0.0011,  3.9757,
  89 (0800): 0.0395, 0.0345, 0.0743, 0.0089, 0.0035,  7.1718,
 105 (0816): 0.0757, 0.0771, 0.1567, 0.0257, 0.0085, 10.8453,
 121 (0832): 0.1201, 0.1398, 0.2693, 0.0578, 0.0166, 14.5406,
 137 (0848): 0.1696, 0.2214, 0.4066, 0.1101, 0.0281, 18.1387,
 153 (0904): 0.2069, 0.2955, 0.5202, 0.1720, 0.0397, 20.7883,
 169 (0920): 0.2542, 0.3946, 0.6693, 0.2628, 0.0557, 23.8007,
 185 (0936): 0.2996, 0.4992, 0.8197, 0.3730, 0.0736, 26.5668,
 201 (0952): 0.3425, 0.6058, 0.9670, 0.4995, 0.0928, 29.1052,
 217 (1008): 0.3802, 0.7061, 1.1005, 0.6330, 0.1118, 31.3284,
 233 (1024): 0.4142, 0.8006, 1.2226, 0.7708, 0.1303, 33.3626,
 249 (1040): 0.4463, 0.8927, 1.3392, 0.9135, 0.1489, 35.3009,
 265 (1056): 0.4734, 0.9729, 1.4381, 1.0485, 0.1657, 37.0183,
 281 (1112): 0.4905, 1.0325, 1.5066, 1.1626, 0.1791, 37.9468,
 297 (1128): 0.4990, 1.0741, 1.5495, 1.2551, 0.1892, 38.1262,
 313 (1144): 0.5066, 1.1097, 1.5860, 1.3373, 0.1979, 38.3779,
 329 (1200): 0.5188, 1.1557, 1.6381, 1.4290, 0.2084, 38.9401,
 345 (1216): 0.5295, 1.1949, 1.6825, 1.5079, 0.2173, 39.4800,
 361 (1232): 0.5383, 1.2264, 1.7183, 1.5721, 0.2246, 39.9548,
 377 (1248): 0.5449, 1.2500, 1.7451, 1.6203, 0.2300, 40.3316,
 393 (1304): 0.5138, 1.1817, 1.6463, 1.5421, 0.2180, 38.1802,
 409 (1320): 0.5139, 1.1826, 1.6466, 1.5466, 0.2184, 38.2155,
 425 (1336): 0.5117, 1.1753, 1.6377, 1.5342, 0.2169, 38.1068,
 441 (1352): 0.5071, 1.1601, 1.6197, 1.5051, 0.2135, 37.8479,
 457 (1408): 0.5001, 1.1370, 1.5927, 1.4600, 0.2083, 37.4378,
 473 (1424): 0.4908, 1.1062, 1.5567, 1.3996, 0.2014, 36.8807,
 489 (1440): 0.4792, 1.0679, 1.5120, 1.3253, 0.1929, 36.1855,
 505 (1456): 0.4654, 1.0226, 1.4589, 1.2384, 0.1828, 35.3656,
 521 (1512): 0.5006, 1.0724, 1.5444, 1.2602, 0.1893, 39.4381,
 537 (1528): 0.4793, 1.0043, 1.4627, 1.1382, 0.1746, 38.2106,
 553 (1544): 0.4574, 0.9337, 1.3778, 1.0138, 0.1595, 36.9775,
 569 (1600): 0.4351, 0.8618, 1.2912, 0.8899, 0.1442, 35.7952,
 585 (1616): 0.4122, 0.7872, 1.2008, 0.7661, 0.1286, 34.7015,
 601 (1632): 0.3860, 0.7074, 1.1012, 0.6425, 0.1125, 33.3564,
 617 (1648): 0.3524, 0.6172, 0.9830, 0.5172, 0.0951, 31.2614,
 633 (1704): 0.3147, 0.5226, 0.8544, 0.3986, 0.0776, 28.8942,
 649 (1720): 0.2736, 0.4266, 0.7187, 0.2915, 0.0608, 26.2581,
 665 (1736): 0.2297, 0.3327, 0.5802, 0.2000, 0.0452, 23.3606,
 681 (1752): 0.1838, 0.2441, 0.4427, 0.1262, 0.0314, 20.1764,
 697 (1808): 0.1296, 0.1593, 0.3021, 0.0690, 0.0193, 14.3998,
 713 (1824): 0.0895, 0.0980, 0.1954, 0.0345, 0.0110, 11.3788,
 729 (1840): 0.0538, 0.0515, 0.1087, 0.0141, 0.0054,  8.2635,
 745 (1856): 0.0268, 0.0223, 0.0498, 0.0045, 0.0021,  5.3751;
ENDX;
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August 22, 1984

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("NO2")
("HCHOr")
("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
LIGHT=6#
   0 (0642): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
  10 (0652): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0254,
  26 (0708): 0.0004, 0.0002, 0.0007, 0.0001, 0.0001,  0.4324,
  42 (0724): 0.0039, 0.0028, 0.0071, 0.0002, 0.0002,  1.7312,
  58 (0740): 0.0141, 0.0108, 0.0252, 0.0016, 0.0009,  3.9128,
  74 (0756): 0.0357, 0.0307, 0.0676, 0.0066, 0.0030,  6.8977,
  90 (0812): 0.0692, 0.0682, 0.1415, 0.0197, 0.0072, 10.3514,
 106 (0828): 0.1118, 0.1253, 0.2466, 0.0462, 0.0144, 13.9499,
 122 (0844): 0.1586, 0.1993, 0.3733, 0.0900, 0.0245, 17.3689,
 138 (0900): 0.2095, 0.2893, 0.5186, 0.1553, 0.0378, 21.2425,
 154 (0916): 0.2589, 0.3897, 0.6720, 0.2424, 0.0537, 24.3389,
 170 (0932): 0.3072, 0.4975, 0.8292, 0.3508, 0.0718, 27.2456,
 186 (0948): 0.3530, 0.6085, 0.9845, 0.4775, 0.0915, 29.9290,
 202 (1004): 0.3951, 0.7178, 1.1319, 0.6170, 0.1118, 32.3829,
 218 (1020): 0.4316, 0.8181, 1.2624, 0.7596, 0.1313, 34.5579,
 234 (1036): 0.4661, 0.9159, 1.3870, 0.9082, 0.1509, 36.6485,
 250 (1052): 0.4993, 1.0113, 1.5070, 1.0607, 0.1704, 38.7290,
 266 (1108): 0.5200, 1.0822, 1.5900, 1.1902, 0.1859, 39.7952,
 282 (1124): 0.5291, 1.1273, 1.6364, 1.2900, 0.1968, 39.9884,
 298 (1140): 0.5357, 1.1634, 1.6719, 1.3760, 0.2059, 40.0991,
 314 (1156): 0.5413, 1.1929, 1.7005, 1.4494, 0.2135, 40.2999,
 330 (1212): 0.5419, 1.2261, 1.7361, 1.5225, 0.2215, 37.8620,
 346 (1228): 0.5503, 1.2580, 1.7718, 1.5886, 0.2289, 38.2769,
 362 (1244): 0.5566, 1.2815, 1.7980, 1.6377, 0.2343, 38.6063,
 378 (1300): 0.5606, 1.2962, 1.8144, 1.6689, 0.2377, 38.8242,
 394 (1316): 0.5620, 1.3017, 1.8204, 1.6811, 0.2391, 38.9091,
 410 (1332): 0.5609, 1.2981, 1.8162, 1.6743, 0.2383, 38.8504,
 426 (1348): 0.5572, 1.2856, 1.8017, 1.6486, 0.2354, 38.6410,
 442 (1404): 0.5509, 1.2640, 1.7770, 1.6046, 0.2305, 38.2790,
 458 (1420): 0.5420, 1.2337, 1.7422, 1.5432, 0.2236, 37.7678,
 474 (1436): 0.5307, 1.1949, 1.6974, 1.4654, 0.2147, 37.1158,
 490 (1452): 0.5132, 1.1373, 1.6288, 1.3599, 0.2022, 36.1761,
 506 (1508): 0.4997, 1.0756, 1.5553, 1.2468, 0.1888, 37.1621,
 522 (1524): 0.4799, 1.0106, 1.4780, 1.1284, 0.1747, 36.0709,
 538 (1540): 0.4592, 0.9424, 1.3968, 1.0065, 0.1599, 34.9722,
 554 (1556): 0.4400, 0.8770, 1.3199, 0.8890, 0.1457, 34.0064,
 570 (1612): 0.4186, 0.8044, 1.2330, 0.7663, 0.1304, 33.0638,
 586 (1628): 0.3930, 0.7240, 1.1333, 0.6413, 0.1140, 31.8464,
 602 (1644): 0.3602, 0.6341, 1.0160, 0.5159, 0.0966, 29.9398,
 618 (1700): 0.3224, 0.5377, 0.8853, 0.3960, 0.0789, 27.7358,
 634 (1716): 0.2806, 0.4391, 0.7459, 0.2877, 0.0617, 25.2562,
 650 (1732): 0.2350, 0.3410, 0.6003, 0.1946, 0.0455, 22.4671,
 666 (1748): 0.1873, 0.2488, 0.4563, 0.1207, 0.0314, 19.4056,
 682 (1804): 0.1383, 0.1679, 0.3225, 0.0672, 0.0198, 15.2631,
 698 (1820): 0.0938, 0.1014, 0.2050, 0.0323, 0.0111, 11.9975,
 714 (1836): 0.0548, 0.0520, 0.1113, 0.0126, 0.0052,  8.6386,
 730 (1852): 0.0261, 0.0219, 0.0497, 0.0037, 0.0020,  5.5400;
ENDX;
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August 25, 1984
("NO2")
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("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
LIGHT=6#
    0 (0644): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
    8 (0652): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0929,
   24 (0708): 0.0007, 0.0004, 0.0014, 0.0001, 0.0001,  0.2907,
   40 (0724): 0.0027, 0.0024, 0.0061, 0.0002, 0.0002,  0.6537,
   56 (0740): 0.0068, 0.0062, 0.0142, 0.0009, 0.0005,  1.1642,
   72 (0756): 0.0145, 0.0143, 0.0311, 0.0030, 0.0014,  1.8253,
   88 (0812): 0.0255, 0.0282, 0.0581, 0.0081, 0.0030,  2.5661,
  104 (0828): 0.0391, 0.0483, 0.0946, 0.0177, 0.0055,  3.3313,
  120 (0844): 0.0534, 0.0732, 0.1368, 0.0329, 0.0090,  4.0486,
  136 (0900): 0.2186, 0.3041, 0.5444, 0.1627, 0.0397, 21.5656,
  152 (0916): 0.2662, 0.4022, 0.6931, 0.2494, 0.0553, 24.4913,
  168 (0932): 0.3113, 0.5048, 0.8412, 0.3548, 0.0728, 27.1552,
  184 (0948): 0.3537, 0.6097, 0.9866, 0.4770, 0.0915, 29.6149,
  200 (1004): 0.3931, 0.7133, 1.1253, 0.6114, 0.1109, 31.8858,
  216 (1020): 0.4282, 0.8110, 1.2517, 0.7511, 0.1300, 33.9557,
  232 (1036): 0.4613, 0.9056, 1.3718, 0.8962, 0.1491, 35.9473,
  248 (1052): 0.4911, 0.9954, 1.4831, 1.0422, 0.1676, 37.7040,
  264 (1108): 0.5119, 1.0664, 1.5664, 1.1712, 0.1831, 38.7685,
  280 (1124): 0.5214, 1.1112, 1.6128, 1.2700, 0.1939, 39.0630,
  296 (1140): 0.5269, 1.1451, 1.6452, 1.3528, 0.2026, 39.1027,
  312 (1156): 0.5315, 1.1719, 1.6703, 1.4224, 0.2097, 39.2316,
  328 (1212): 0.5501, 1.2302, 1.7420, 1.5257, 0.2221, 40.0730,
  344 (1228): 0.5580, 1.2608, 1.7757, 1.5900, 0.2292, 40.4702,
  360 (1244): 0.5639, 1.2830, 1.8002, 1.6373, 0.2345, 40.7827,
  376 (1300): 0.5674, 1.2965, 1.8150, 1.6667, 0.2377, 40.9833,
  392 (1316): 0.5682, 1.3001, 1.8186, 1.6758, 0.2386, 41.0442,
  408 (1332): 0.5666, 1.2949, 1.8123, 1.6663, 0.2375, 40.9604,
  424 (1348): 0.5625, 1.2808, 1.7961, 1.6382, 0.2343, 40.7244,
  440 (1404): 0.5558, 1.2581, 1.7700, 1.5921, 0.2291, 40.3343,
  456 (1420): 0.5467, 1.2268, 1.7341, 1.5288, 0.2220, 39.7935,
  472 (1436): 0.5334, 1.1823, 1.6819, 1.4435, 0.2121, 39.0311,
  488 (1452): 0.5154, 1.1236, 1.6119, 1.3365, 0.1994, 38.0346,
  504 (1508): 0.4243, 0.9169, 1.3285, 1.0564, 0.1605, 30.2697,
  520 (1524): 0.4075, 0.8609, 1.2620, 0.9546, 0.1484, 29.3902,
  536 (1540): 0.3907, 0.8038, 1.1945, 0.8517, 0.1360, 28.5352,
  552 (1556): 0.3743, 0.7474, 1.1282, 0.7506, 0.1237, 27.7643,
  568 (1612): 0.3566, 0.6859, 1.0549, 0.6466, 0.1107, 27.0357,
  584 (1628): 0.3351, 0.6178, 0.9706, 0.5407, 0.0968, 26.0450,
  600 (1644): 0.3083, 0.5428, 0.8732, 0.4355, 0.0823, 24.5607,
  616 (1700): 0.2770, 0.4618, 0.7636, 0.3347, 0.0673, 22.8275,
  632 (1716): 0.2421, 0.3785, 0.6459, 0.2434, 0.0528, 20.8626,
  648 (1732): 0.2036, 0.2949, 0.5218, 0.1648, 0.0391, 18.6237,
  664 (1748): 0.1633, 0.2167, 0.3994, 0.1026, 0.0271, 16.1728,
  680 (1804): 0.1515, 0.1829, 0.3528, 0.0712, 0.0214, 16.3890,
  696 (1820): 0.1035, 0.1117, 0.2266, 0.0344, 0.0121, 12.9675,
  712 (1836): 0.0617, 0.0592, 0.1268, 0.0137, 0.0059,  9.4926,
  728 (1852): 0.0307, 0.0268, 0.0606, 0.0043, 0.0024,  6.2864;
ENDX;
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September 1, 1984

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("NO2")
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("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
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  11 (0700): 0.0003, 0.0001, 0.0004, 0.0001, 0.0001,  1.1321,
  27 (0716): 0.0055, 0.0038, 0.0110, 0.0002, 0.0002,  2.6788,
  43 (0732): 0.0159, 0.0133, 0.0323, 0.0013, 0.0010,  5.0775,
  59 (0748): 0.0368, 0.0315, 0.0712, 0.0050, 0.0028,  8.3748,
  75 (0804): 0.0725, 0.0685, 0.1462, 0.0159, 0.0068, 12.4185,
  91 (0820): 0.1196, 0.1272, 0.2566, 0.0394, 0.0138, 16.7291,
 107 (0836): 0.1736, 0.2065, 0.3957, 0.0812, 0.0243, 21.0063,
 123 (0852): 0.2290, 0.3008, 0.5507, 0.1444, 0.0378, 24.9736,
 139 (0908): 0.2672, 0.3865, 0.6791, 0.2191, 0.0515, 26.1282,
 155 (0924): 0.3181, 0.4964, 0.8413, 0.3240, 0.0697, 29.2964,
 171 (0940): 0.3658, 0.6090, 1.0001, 0.4479, 0.0894, 32.1921,
 187 (0956): 0.4106, 0.7224, 1.1541, 0.5881, 0.1102, 34.8892,
 203 (1012): 0.4517, 0.8325, 1.2988, 0.7385, 0.1313, 37.4014,
 219 (1028): 0.4897, 0.9381, 1.4341, 0.8952, 0.1522, 39.7913,
 235 (1044): 0.5222, 1.0361, 1.5557, 1.0523, 0.1724, 41.6584,
 251 (1100): 0.5494, 1.1242, 1.6617, 1.2037, 0.1911, 43.1272,
 267 (1116): 0.5707, 1.1968, 1.7461, 1.3394, 0.2071, 44.3235,
 283 (1132): 0.5793, 1.2403, 1.7897, 1.4398, 0.2179, 44.5685,
 299 (1148): 0.5834, 1.2699, 1.8161, 1.5192, 0.2259, 44.5548,
 315 (1204): 0.5623, 1.2480, 1.7721, 1.5294, 0.2243, 41.6666,
 331 (1220): 0.5665, 1.2696, 1.7927, 1.5852, 0.2299, 41.8638,
 347 (1236): 0.5716, 1.2909, 1.8151, 1.6344, 0.2351, 42.1318,
 363 (1252): 0.5758, 1.3071, 1.8326, 1.6701, 0.2390, 42.3576,
 379 (1308): 0.5775, 1.3143, 1.8402, 1.6869, 0.2408, 42.4584,
 395 (1324): 0.5767, 1.3125, 1.8376, 1.6844, 0.2404, 42.4160,
 411 (1340): 0.5734, 1.3015, 1.8248, 1.6627, 0.2380, 42.2188,
 427 (1356): 0.5675, 1.2814, 1.8017, 1.6221, 0.2334, 41.8621,
 443 (1412): 0.5576, 1.2487, 1.7635, 1.5585, 0.2261, 41.2878,
 459 (1428): 0.5433, 1.2017, 1.7076, 1.4711, 0.2158, 40.4690,
 475 (1444): 0.5259, 1.1452, 1.6403, 1.3675, 0.2035, 39.4854,
 491 (1500): 0.5065, 1.0821, 1.5649, 1.2531, 0.1899, 38.3926,
 507 (1516): 0.4866, 1.0188, 1.4902, 1.1368, 0.1760, 37.0316,
 523 (1532): 0.4674, 0.9544, 1.4144, 1.0189, 0.1620, 35.9863,
 539 (1548): 0.4478, 0.8881, 1.3365, 0.8997, 0.1476, 34.9883,
 555 (1604): 0.4271, 0.8175, 1.2526, 0.7784, 0.1325, 34.0403,
 571 (1620): 0.4042, 0.7413, 1.1601, 0.6561, 0.1167, 33.0796,
 587 (1636): 0.3735, 0.6554, 1.0497, 0.5326, 0.0999, 31.2807,
 603 (1652): 0.3382, 0.5635, 0.9269, 0.4141, 0.0826, 29.2121,
 619 (1708): 0.2980, 0.4666, 0.7916, 0.3046, 0.0655, 26.8239,
 635 (1724): 0.2523, 0.3670, 0.6452, 0.2082, 0.0489, 24.0487,
 651 (1740): 0.2043, 0.2727, 0.4993, 0.1310, 0.0343, 21.0021,
 667 (1756): 0.1556, 0.1884, 0.3611, 0.0743, 0.0222, 17.7164,
 683 (1812): 0.1272, 0.1404, 0.2832, 0.0437, 0.0153, 15.6041,
 699 (1828): 0.0762, 0.0748, 0.1595, 0.0174, 0.0074, 11.4953,
 715 (1844): 0.0381, 0.0339, 0.0765, 0.0054, 0.0030,  7.6841,
 731 (1900): 0.0161, 0.0140, 0.0340, 0.0013, 0.0011,  4.5714;
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September 2, 1984

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("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
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  10 (0700): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0540,
  26 (0716): 0.0010, 0.0005, 0.0016, 0.0001, 0.0001,  0.8882,
  42 (0732): 0.0068, 0.0050, 0.0126, 0.0005, 0.0004,  2.9500,
  58 (0748): 0.0221, 0.0173, 0.0398, 0.0027, 0.0015,  6.1336,
  74 (0804): 0.0519, 0.0460, 0.0994, 0.0104, 0.0045, 10.2264,
  90 (0820): 0.0948, 0.0963, 0.1963, 0.0292, 0.0104, 14.7093,
 106 (0836): 0.1463, 0.1685, 0.3255, 0.0650, 0.0197, 19.1888,
 122 (0852): 0.2015, 0.2589, 0.4765, 0.1224, 0.0324, 23.4184,
 138 (0908): 0.2362, 0.3400, 0.5995, 0.1906, 0.0452, 23.4330,
 154 (0924): 0.2869, 0.4475, 0.7600, 0.2896, 0.0626, 26.6040,
 170 (0940): 0.3346, 0.5582, 0.9178, 0.4080, 0.0817, 29.4957,
 186 (0956): 0.3793, 0.6699, 1.0710, 0.5428, 0.1020, 32.1809,
 202 (1012): 0.4195, 0.7765, 1.2119, 0.6863, 0.1223, 34.6387,
 218 (1028): 0.4567, 0.8786, 1.3437, 0.8359, 0.1424, 36.9805,
 234 (1044): 0.4877, 0.9724, 1.4602, 0.9851, 0.1617, 38.7156,
 250 (1100): 0.5141, 1.0573, 1.5629, 1.1296, 0.1796, 40.1477,
 266 (1116): 0.5358, 1.1294, 1.6477, 1.2617, 0.1954, 41.3577,
 282 (1132): 0.5451, 1.1728, 1.6923, 1.3593, 0.2060, 41.6808,
 298 (1148): 0.5491, 1.2016, 1.7182, 1.4353, 0.2137, 41.6787,
 314 (1204): 0.5420, 1.2030, 1.7081, 1.4723, 0.2161, 40.6749,
 330 (1220): 0.5464, 1.2246, 1.7291, 1.5271, 0.2217, 40.8845,
 346 (1236): 0.5510, 1.2443, 1.7495, 1.5733, 0.2266, 41.1332,
 362 (1252): 0.5551, 1.2602, 1.7669, 1.6081, 0.2303, 41.3571,
 378 (1308): 0.5568, 1.2674, 1.7744, 1.6244, 0.2321, 41.4553,
 394 (1324): 0.5561, 1.2655, 1.7718, 1.6218, 0.2317, 41.4091,
 410 (1340): 0.5527, 1.2546, 1.7591, 1.6004, 0.2293, 41.2068,
 426 (1356): 0.5468, 1.2348, 1.7362, 1.5605, 0.2248, 40.8435,
 442 (1412): 0.5364, 1.2007, 1.6960, 1.4958, 0.2173, 40.2365,
 458 (1428): 0.5223, 1.1549, 1.6415, 1.4107, 0.2072, 39.4235,
 474 (1444): 0.5053, 1.0998, 1.5757, 1.3101, 0.1953, 38.4475,
 490 (1500): 0.4862, 1.0380, 1.5018, 1.1986, 0.1819, 37.3579,
 506 (1516): 0.4725, 0.9891, 1.4474, 1.1001, 0.1707, 36.3513,
 522 (1532): 0.4534, 0.9258, 1.3728, 0.9846, 0.1569, 35.2983,
 538 (1548): 0.4336, 0.8598, 1.2947, 0.8672, 0.1426, 34.2749,
 554 (1604): 0.4126, 0.7893, 1.2104, 0.7475, 0.1277, 33.2983,
 570 (1620): 0.3889, 0.7124, 1.1161, 0.6263, 0.1119, 32.2682,
 586 (1636): 0.3571, 0.6254, 1.0031, 0.5040, 0.0950, 30.3726,
 602 (1652): 0.3208, 0.5328, 0.8782, 0.3876, 0.0779, 28.2038,
 618 (1708): 0.2799, 0.4364, 0.7422, 0.2812, 0.0610, 25.7229,
 634 (1724): 0.2338, 0.3378, 0.5960, 0.1885, 0.0448, 22.8546,
 650 (1740): 0.1859, 0.2459, 0.4524, 0.1157, 0.0307, 19.7294,
 666 (1756): 0.1381, 0.1650, 0.3182, 0.0633, 0.0192, 16.3776,
 682 (1812): 0.0902, 0.0975, 0.1985, 0.0292, 0.0105, 11.7120,
 698 (1828): 0.0512, 0.0487, 0.1051, 0.0108, 0.0048,  8.3474,
 714 (1844): 0.0233, 0.0198, 0.0455, 0.0030, 0.0017,  5.2543,
 730 (1900): 0.0083, 0.0067, 0.0167, 0.0006, 0.0005,  2.7911;
ENDX;
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September 3, 1984

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("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
LIGHT=6#
   0 (0651): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
   9 (0700): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0373,
  25 (0716): 0.0006, 0.0004, 0.0011, 0.0001, 0.0001,  0.5668,
  41 (0732): 0.0052, 0.0040, 0.0100, 0.0003, 0.0003,  2.0661,
  57 (0748): 0.0185, 0.0150, 0.0348, 0.0023, 0.0013,  4.5384,
  73 (0804): 0.0460, 0.0423, 0.0920, 0.0094, 0.0041,  7.8334,
  89 (0820): 0.0871, 0.0920, 0.1884, 0.0275, 0.0099, 11.5383,
 105 (0836): 0.1379, 0.1657, 0.3209, 0.0634, 0.0193, 15.3245,
 121 (0852): 0.1923, 0.2581, 0.4759, 0.1213, 0.0322, 18.8860,
 137 (0908): 0.2202, 0.3219, 0.5682, 0.1797, 0.0427, 20.5749,
 153 (0924): 0.2691, 0.4269, 0.7253, 0.2757, 0.0597, 23.4634,
 169 (0940): 0.3161, 0.5372, 0.8831, 0.3922, 0.0786, 26.1456,
 185 (0956): 0.3607, 0.6498, 1.0382, 0.5265, 0.0990, 28.6650,
 201 (1012): 0.4013, 0.7581, 1.1822, 0.6707, 0.1195, 30.9808,
 217 (1028): 0.4390, 0.8628, 1.3177, 0.8223, 0.1400, 33.2007,
 233 (1044): 0.4697, 0.9578, 1.4359, 0.9727, 0.1594, 34.7607,
 249 (1100): 0.4965, 1.0448, 1.5415, 1.1195, 0.1777, 36.1199,
 265 (1116): 0.5191, 1.1207, 1.6315, 1.2561, 0.1942, 37.2984,
 281 (1132): 0.5295, 1.1671, 1.6802, 1.3575, 0.2053, 37.6860,
 297 (1148): 0.5340, 1.1972, 1.7078, 1.4355, 0.2133, 37.6970,
 313 (1204): 0.5387, 1.2238, 1.7330, 1.5035, 0.2202, 37.8456,
 329 (1220): 0.5436, 1.2473, 1.7564, 1.5617, 0.2263, 38.0613,
 345 (1236): 0.5482, 1.2674, 1.7771, 1.6091, 0.2312, 38.2905,
 361 (1252): 0.4852, 1.1309, 1.5811, 1.4491, 0.2071, 33.4396,
 377 (1308): 0.4869, 1.1377, 1.5884, 1.4645, 0.2088, 33.5219,
 393 (1324): 0.4862, 1.1361, 1.5861, 1.4621, 0.2085, 33.4803,
 409 (1340): 0.4832, 1.1263, 1.5748, 1.4427, 0.2063, 33.3120,
 425 (1356): 0.4779, 1.1083, 1.5541, 1.4062, 0.2022, 33.0083,
 441 (1412): 0.4685, 1.0766, 1.5166, 1.3463, 0.1952, 32.4969,
 457 (1428): 0.4563, 1.0359, 1.4685, 1.2701, 0.1863, 31.8407,
 473 (1444): 0.4416, 0.9871, 1.4104, 1.1799, 0.1756, 31.0542,
 489 (1500): 0.4250, 0.9320, 1.3449, 1.0798, 0.1637, 30.1736,
 505 (1516): 0.4190, 0.9042, 1.3196, 1.0085, 0.1563, 29.3104,
 521 (1532): 0.4024, 0.8476, 1.2534, 0.9038, 0.1439, 28.4673,
 537 (1548): 0.3851, 0.7878, 1.1832, 0.7963, 0.1309, 27.6405,
 553 (1604): 0.3667, 0.7238, 1.1072, 0.6866, 0.1172, 26.8567,
 569 (1620): 0.3456, 0.6534, 1.0213, 0.5748, 0.1027, 26.0063,
 585 (1636): 0.3168, 0.5729, 0.9170, 0.4615, 0.0871, 24.4342,
 601 (1652): 0.2842, 0.4875, 0.8020, 0.3539, 0.0712, 22.6425,
 617 (1708): 0.2474, 0.3986, 0.6769, 0.2558, 0.0556, 20.6037,
 633 (1724): 0.2061, 0.3078, 0.5425, 0.1706, 0.0407, 18.2591,
 649 (1740): 0.1634, 0.2233, 0.4107, 0.1039, 0.0278, 15.7138,
 665 (1756): 0.1208, 0.1490, 0.2876, 0.0562, 0.0173, 12.9900,
 681 (1812): 0.0154, 0.0188, 0.0383, 0.0055, 0.0020,  1.0503,
 697 (1828): 0.0086, 0.0092, 0.0201, 0.0020, 0.0009,  0.7392,
 713 (1844): 0.0038, 0.0036, 0.0084, 0.0005, 0.0003,  0.4544,
 729 (1900): 0.0013, 0.0011, 0.0029, 0.0001, 0.0001,  0.2313;
ENDX;
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September 8, 1984

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("NO2")
("HCHOr")
("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
LIGHT=6#
   0 (0654): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
  10 (0704): 0.0009, 0.0005, 0.0017, 0.0001, 0.0001,  2.8046,
  26 (0720): 0.0102, 0.0077, 0.0219, 0.0003, 0.0005,  3.9243,
  42 (0736): 0.0229, 0.0208, 0.0501, 0.0020, 0.0016,  6.2528,
  58 (0752): 0.0463, 0.0423, 0.0943, 0.0069, 0.0038,  9.5532,
  74 (0808): 0.0855, 0.0846, 0.1786, 0.0199, 0.0085, 13.5687,
  90 (0824): 0.1360, 0.1498, 0.2998, 0.0472, 0.0164, 17.8075,
 106 (0840): 0.1929, 0.2365, 0.4502, 0.0944, 0.0280, 21.9907,
 122 (0856): 0.2510, 0.3386, 0.6162, 0.1646, 0.0428, 25.8769,
 138 (0912): 0.2949, 0.4351, 0.7606, 0.2495, 0.0583, 27.7073,
 154 (0928): 0.3484, 0.5536, 0.9339, 0.3650, 0.0780, 30.8988,
 170 (0944): 0.3982, 0.6739, 1.1021, 0.4999, 0.0993, 33.8148,
 186 (1000): 0.4448, 0.7945, 1.2648, 0.6515, 0.1216, 36.5509,
 202 (1016): 0.4880, 0.9114, 1.4176, 0.8134, 0.1441, 39.1524,
 218 (1032): 0.5243, 1.0198, 1.5540, 0.9782, 0.1659, 41.1264,
 234 (1048): 0.5557, 1.1197, 1.6760, 1.1418, 0.1867, 42.7698,
 250 (1104): 0.5835, 1.2111, 1.7853, 1.3004, 0.2062, 44.2573,
 266 (1120): 0.6077, 1.2930, 1.8816, 1.4498, 0.2241, 45.5770,
 282 (1136): 0.6164, 1.3364, 1.9247, 1.5525, 0.2350, 45.8988,
 298 (1152): 0.6190, 1.3638, 1.9471, 1.6306, 0.2427, 45.7680,
 314 (1208): 0.6131, 1.3783, 1.9545, 1.6862, 0.2476, 43.7431,
 330 (1224): 0.6165, 1.3987, 1.9731, 1.7412, 0.2531, 43.8675,
 346 (1240): 0.6195, 1.4146, 1.9883, 1.7831, 0.2573, 44.0043,
 362 (1256): 0.6214, 1.4250, 1.9982, 1.8098, 0.2600, 44.0989,
 378 (1312): 0.6216, 1.4275, 2.0000, 1.8181, 0.2608, 44.0987,
 394 (1328): 0.6188, 1.4194, 1.9899, 1.8043, 0.2591, 43.9418,
 410 (1344): 0.6121, 1.3976, 1.9637, 1.7646, 0.2544, 43.5720,
 426 (1400): 0.6024, 1.3655, 1.9256, 1.7041, 0.2473, 43.0310,
 442 (1416): 0.5892, 1.3219, 1.8741, 1.6223, 0.2377, 42.3024,
 458 (1432): 0.5728, 1.2676, 1.8098, 1.5214, 0.2258, 41.3971,
 474 (1448): 0.5534, 1.2034, 1.7334, 1.4042, 0.2119, 40.3346,
 490 (1504): 0.5341, 1.1405, 1.6605, 1.2856, 0.1980, 38.8819,
 506 (1520): 0.5150, 1.0754, 1.5847, 1.1631, 0.1835, 37.8606,
 522 (1536): 0.4950, 1.0062, 1.5041, 1.0360, 0.1684, 36.8422,
 538 (1552): 0.4737, 0.9323, 1.4172, 0.9053, 0.1524, 35.8502,
 554 (1608): 0.4512, 0.8535, 1.3235, 0.7733, 0.1357, 34.9606,
 570 (1624): 0.4237, 0.7674, 1.2171, 0.6409, 0.1182, 33.6446,
 586 (1640): 0.3885, 0.6704, 1.0905, 0.5086, 0.0996, 31.6784,
 602 (1656): 0.3483, 0.5679, 0.9512, 0.3848, 0.0809, 29.4270,
 618 (1712): 0.3018, 0.4598, 0.7966, 0.2724, 0.0623, 26.7836,
 634 (1728): 0.2507, 0.3528, 0.6353, 0.1782, 0.0452, 23.7846,
 650 (1744): 0.1978, 0.2543, 0.4783, 0.1062, 0.0305, 20.5185,
 666 (1800): 0.1435, 0.1664, 0.3289, 0.0553, 0.0185, 16.8856,
 682 (1816): 0.0909, 0.0958, 0.1997, 0.0241, 0.0098, 12.1977,
 698 (1832): 0.0508, 0.0488, 0.1075, 0.0086, 0.0045,  8.7404,
 714 (1848): 0.0251, 0.0236, 0.0557, 0.0026, 0.0019,  5.7818;
ENDX;
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September 17, 1984

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("HCHOs")
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("CCHO ")
("O3=O(3P)")
LIGHT=6#
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  11 (0712): 0.0034, 0.0023, 0.0071, 0.0001, 0.0001,  5.0085,
  27 (0728): 0.0176, 0.0149, 0.0406, 0.0008, 0.0010,  5.2681,
  43 (0744): 0.0317, 0.0305, 0.0716, 0.0032, 0.0024,  7.5807,
  59 (0800): 0.0587, 0.0566, 0.1238, 0.0099, 0.0052, 10.9660,
  75 (0816): 0.1013, 0.1056, 0.2188, 0.0265, 0.0108, 14.9527,
  91 (0832): 0.1542, 0.1781, 0.3502, 0.0594, 0.0199, 19.1246,
 107 (0848): 0.2115, 0.2703, 0.5061, 0.1135, 0.0325, 23.1607,
 123 (0904): 0.2677, 0.3742, 0.6710, 0.1901, 0.0481, 26.8212,
 139 (0920): 0.3227, 0.4882, 0.8423, 0.2909, 0.0664, 30.2433,
 155 (0936): 0.3757, 0.6090, 1.0155, 0.4149, 0.0870, 33.4683,
 171 (0952): 0.4245, 0.7293, 1.1810, 0.5563, 0.1086, 36.4444,
 187 (1008): 0.4685, 0.8465, 1.3360, 0.7105, 0.1308, 39.0627,
 203 (1024): 0.5056, 0.9555, 1.4744, 0.8696, 0.1523, 41.0541,
 219 (1040): 0.5389, 1.0578, 1.6010, 1.0309, 0.1733, 42.8772,
 235 (1056): 0.5685, 1.1521, 1.7149, 1.1893, 0.1931, 44.5217,
 251 (1112): 0.5447, 1.1585, 1.7003, 1.2550, 0.1980, 38.7287,
 267 (1128): 0.5627, 1.2223, 1.7734, 1.3780, 0.2124, 39.7106,
 283 (1144): 0.5712, 1.2627, 1.8145, 1.4706, 0.2223, 40.0428,
 299 (1200): 0.5722, 1.2834, 1.8299, 1.5340, 0.2284, 39.8630,
 315 (1216): 0.6302, 1.4183, 2.0104, 1.7297, 0.2545, 45.0417,
 331 (1232): 0.6315, 1.4318, 2.0208, 1.7716, 0.2585, 45.0430,
 347 (1248): 0.6317, 1.4390, 2.0255, 1.7973, 0.2608, 45.0249,
 363 (1304): 0.6304, 1.4384, 2.0222, 1.8043, 0.2612, 44.9325,
 379 (1320): 0.6253, 1.4245, 2.0036, 1.7852, 0.2585, 44.6658,
 395 (1336): 0.6161, 1.3960, 1.9680, 1.7392, 0.2527, 44.1847,
 411 (1352): 0.6048, 1.3599, 1.9241, 1.6757, 0.2450, 43.5757,
 427 (1408): 0.5925, 1.3189, 1.8756, 1.5993, 0.2360, 42.8797,
 443 (1424): 0.5767, 1.2668, 1.8139, 1.5030, 0.2247, 42.0035,
 459 (1440): 0.5578, 1.2044, 1.7396, 1.3897, 0.2111, 40.9629,
 475 (1456): 0.5374, 1.1371, 1.6597, 1.2677, 0.1965, 39.8527,
 491 (1512): 0.5018, 1.0332, 1.5268, 1.1048, 0.1756, 38.1665,
 507 (1528): 0.4823, 0.9666, 1.4489, 0.9835, 0.1610, 37.1360,
 523 (1544): 0.4611, 0.8946, 1.3640, 0.8579, 0.1455, 36.1102,
 539 (1600): 0.4401, 0.8214, 1.2773, 0.7344, 0.1300, 35.2218,
 555 (1616): 0.4152, 0.7407, 1.1785, 0.6094, 0.1135, 34.1429,
 571 (1632): 0.3810, 0.6473, 1.0566, 0.4829, 0.0956, 32.1881,
 587 (1648): 0.3414, 0.5477, 0.9208, 0.3638, 0.0774, 29.9131,
 603 (1704): 0.2957, 0.4431, 0.7709, 0.2564, 0.0596, 27.2440,
 619 (1720): 0.2465, 0.3415, 0.6177, 0.1677, 0.0434, 24.2723,
 635 (1736): 0.1944, 0.2463, 0.4655, 0.0994, 0.0293, 20.9631,
 651 (1752): 0.1401, 0.1605, 0.3186, 0.0510, 0.0176, 17.2078,
 667 (1808): 0.0912, 0.0970, 0.2031, 0.0230, 0.0097, 12.2823,
 683 (1824): 0.0517, 0.0513, 0.1135, 0.0083, 0.0046,  8.8847,
 699 (1840): 0.0282, 0.0282, 0.0674, 0.0027, 0.0022,  6.1032,
 715 (1856): 0.0149, 0.0125, 0.0349, 0.0005, 0.0008,  4.3135;
ENDX;
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September 19, 1984

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("CCHO ")
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   9 (0712): 0.0001, 0.0001, 0.0002, 0.0001, 0.0001,  0.7335,
  25 (0728): 0.0041, 0.0028, 0.0081, 0.0001, 0.0002,  2.1696,
  41 (0744): 0.0153, 0.0129, 0.0318, 0.0012, 0.0010,  4.6762,
  57 (0800): 0.0382, 0.0341, 0.0772, 0.0054, 0.0030,  8.1282,
  73 (0816): 0.0765, 0.0766, 0.1622, 0.0179, 0.0076, 12.2016,
  89 (0832): 0.1260, 0.1427, 0.2846, 0.0450, 0.0156, 16.4297,
 105 (0848): 0.1825, 0.2313, 0.4373, 0.0932, 0.0275, 20.5994,
 121 (0904): 0.2263, 0.3161, 0.5705, 0.1557, 0.0402, 23.0103,
 137 (0920): 0.2800, 0.4250, 0.7367, 0.2473, 0.0573, 26.4237,
 153 (0936): 0.3324, 0.5419, 0.9067, 0.3625, 0.0769, 29.6563,
 169 (0952): 0.3817, 0.6603, 1.0720, 0.4963, 0.0979, 32.6891,
 185 (1008): 0.4247, 0.7741, 1.2239, 0.6420, 0.1191, 35.1655,
 201 (1024): 0.4617, 0.8805, 1.3606, 0.7933, 0.1399, 37.1711,
 217 (1040): 0.4951, 0.9810, 1.4863, 0.9477, 0.1602, 39.0079,
 233 (1056): 0.5248, 1.0738, 1.5998, 1.1000, 0.1795, 40.6673,
 249 (1112): 0.5508, 1.1576, 1.7004, 1.2455, 0.1974, 42.1420,
 265 (1128): 0.5709, 1.2251, 1.7788, 1.3725, 0.2124, 43.3274,
 281 (1144): 0.5831, 1.2735, 1.8313, 1.4745, 0.2238, 43.9405,
 297 (1200): 0.5846, 1.2958, 1.8487, 1.5403, 0.2302, 43.7396,
 313 (1216): 0.5691, 1.2815, 1.8174, 1.5543, 0.2295, 41.5628,
 329 (1232): 0.5706, 1.2945, 1.8279, 1.5931, 0.2333, 41.5760,
 345 (1248): 0.5710, 1.3012, 1.8325, 1.6164, 0.2354, 41.5615,
 361 (1304): 0.5696, 1.3004, 1.8292, 1.6221, 0.2356, 41.4658,
 377 (1320): 0.5646, 1.2864, 1.8106, 1.6029, 0.2330, 41.1911,
 393 (1336): 0.5557, 1.2590, 1.7763, 1.5591, 0.2274, 40.7172,
 409 (1352): 0.5451, 1.2251, 1.7350, 1.5001, 0.2202, 40.1258,
 425 (1408): 0.5334, 1.1873, 1.6901, 1.4300, 0.2120, 39.4492,
 441 (1424): 0.5187, 1.1393, 1.6330, 1.3418, 0.2015, 38.6028,
 457 (1440): 0.5013, 1.0827, 1.5654, 1.2392, 0.1892, 37.6153,
 473 (1456): 0.4824, 1.0210, 1.4920, 1.1281, 0.1759, 36.5492,
 489 (1512): 0.4727, 0.9781, 1.4474, 1.0354, 0.1656, 36.0294,
 505 (1528): 0.4529, 0.9123, 1.3698, 0.9175, 0.1513, 34.9666,
 521 (1544): 0.4316, 0.8414, 1.2853, 0.7961, 0.1362, 33.9118,
 537 (1600): 0.4107, 0.7704, 1.2007, 0.6779, 0.1212, 33.0125,
 553 (1616): 0.3849, 0.6899, 1.1007, 0.5569, 0.1050, 31.8136,
 569 (1632): 0.3496, 0.5966, 0.9771, 0.4349, 0.0874, 29.7436,
 585 (1648): 0.3089, 0.4971, 0.8396, 0.3209, 0.0696, 27.3440,
 601 (1704): 0.2632, 0.3950, 0.6913, 0.2204, 0.0525, 24.5991,
 617 (1720): 0.2145, 0.2968, 0.5412, 0.1390, 0.0371, 21.5628,
 633 (1736): 0.1636, 0.2059, 0.3936, 0.0780, 0.0240, 18.1989,
 649 (1752): 0.1123, 0.1265, 0.2555, 0.0369, 0.0135, 14.4760,
 665 (1808): 0.0634, 0.0645, 0.1387, 0.0136, 0.0062,  9.4739,
 681 (1824): 0.0309, 0.0283, 0.0653, 0.0039, 0.0024,  6.2122,
 697 (1840): 0.0124, 0.0105, 0.0269, 0.0008, 0.0008,  3.5209,
 713 (1856): 0.0027, 0.0017, 0.0051, 0.0001, 0.0001,  1.6156;
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September 21, 1984

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("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
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   8 (0712): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.6846,
  24 (0728): 0.0034, 0.0023, 0.0066, 0.0001, 0.0001,  1.9707,
  40 (0744): 0.0142, 0.0120, 0.0297, 0.0011, 0.0009,  4.3877,
  56 (0800): 0.0361, 0.0323, 0.0734, 0.0049, 0.0028,  7.7544,
  72 (0816): 0.0737, 0.0737, 0.1567, 0.0167, 0.0073, 11.7666,
  88 (0832): 0.1230, 0.1391, 0.2785, 0.0429, 0.0151, 15.9357,
 104 (0848): 0.1798, 0.2278, 0.4319, 0.0901, 0.0269, 20.0915,
 120 (0904): 0.2183, 0.3051, 0.5522, 0.1481, 0.0386, 21.9000,
 136 (0920): 0.2708, 0.4113, 0.7146, 0.2364, 0.0552, 25.1903,
 152 (0936): 0.3219, 0.5252, 0.8807, 0.3476, 0.0742, 28.3098,
 168 (0952): 0.3703, 0.6411, 1.0430, 0.4775, 0.0947, 31.2602,
 184 (1008): 0.4110, 0.7508, 1.1890, 0.6177, 0.1152, 33.4901,
 200 (1024): 0.4471, 0.8544, 1.3223, 0.7642, 0.1354, 35.4299,
 216 (1040): 0.4795, 0.9521, 1.4447, 0.9137, 0.1551, 37.2013,
 232 (1056): 0.5084, 1.0422, 1.5551, 1.0611, 0.1738, 38.7991,
 248 (1112): 0.5334, 1.1229, 1.6519, 1.2011, 0.1910, 40.2064,
 264 (1128): 0.5530, 1.1885, 1.7282, 1.3240, 0.2056, 41.3475,
 280 (1144): 0.5660, 1.2373, 1.7820, 1.4246, 0.2169, 42.0684,
 296 (1200): 0.5676, 1.2602, 1.8005, 1.4899, 0.2234, 41.8530,
 312 (1216): 0.5500, 1.2383, 1.7586, 1.4938, 0.2213, 39.8467,
 328 (1232): 0.5510, 1.2497, 1.7673, 1.5296, 0.2247, 39.8279,
 344 (1248): 0.5509, 1.2549, 1.7701, 1.5502, 0.2265, 39.7834,
 360 (1304): 0.5490, 1.2525, 1.7648, 1.5533, 0.2264, 39.6599,
 376 (1320): 0.5432, 1.2361, 1.7431, 1.5308, 0.2233, 39.3501,
 392 (1336): 0.5337, 1.2068, 1.7061, 1.4845, 0.2174, 38.8502,
 408 (1352): 0.5227, 1.1721, 1.6636, 1.4249, 0.2101, 38.2502,
 424 (1408): 0.5111, 1.1344, 1.6187, 1.3558, 0.2019, 37.5809,
 440 (1424): 0.4965, 1.0869, 1.5620, 1.2695, 0.1916, 36.7497,
 456 (1440): 0.4798, 1.0325, 1.4970, 1.1711, 0.1798, 35.8024,
 472 (1456): 0.4612, 0.9721, 1.4249, 1.0634, 0.1668, 34.7646,
 488 (1512): 0.4400, 0.9136, 1.3566, 0.9564, 0.1540, 32.2447,
 504 (1528): 0.4209, 0.8502, 1.2813, 0.8445, 0.1403, 31.2661,
 520 (1544): 0.4006, 0.7825, 1.2002, 0.7301, 0.1260, 30.3021,
 536 (1600): 0.3805, 0.7142, 1.1184, 0.6186, 0.1117, 29.4737,
 552 (1616): 0.3551, 0.6366, 1.0209, 0.5047, 0.0962, 28.3099,
 568 (1632): 0.3210, 0.5471, 0.9012, 0.3905, 0.0795, 26.3915,
 584 (1648): 0.2815, 0.4515, 0.7676, 0.2844, 0.0627, 24.1551,
 600 (1704): 0.2379, 0.3551, 0.6260, 0.1925, 0.0467, 21.6227,
 616 (1720): 0.1917, 0.2631, 0.4839, 0.1191, 0.0325, 18.8276,
 632 (1736): 0.1436, 0.1787, 0.3450, 0.0650, 0.0205, 15.7250,
 648 (1752): 0.0962, 0.1070, 0.2184, 0.0297, 0.0113, 12.3385,
 664 (1808): 0.0555, 0.0551, 0.1198, 0.0109, 0.0052,  8.7570,
 680 (1824): 0.0260, 0.0234, 0.0548, 0.0030, 0.0020,  5.6125,
 696 (1840): 0.0099, 0.0082, 0.0214, 0.0006, 0.0006,  3.0681,
 712 (1856): 0.0016, 0.0009, 0.0029, 0.0001, 0.0001,  1.3343;
ENDX;
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June 26, 1985

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("NO2")
("HCHOr")
("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
LIGHT=6#
   0 (0602): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
  10 (0612): 0.0001, 0.0001, 0.0002, 0.0001, 0.0001,  0.9021,
  26 (0628): 0.0035, 0.0020, 0.0064, 0.0001, 0.0001,  2.0040,
  42 (0644): 0.0116, 0.0087, 0.0235, 0.0005, 0.0006,  3.8445,
  58 (0700): 0.0266, 0.0209, 0.0512, 0.0021, 0.0016,  6.4742,
  74 (0716): 0.0525, 0.0445, 0.1023, 0.0068, 0.0039,  9.6170,
  90 (0732): 0.0886, 0.0840, 0.1822, 0.0181, 0.0081, 13.1065,
 106 (0748): 0.1322, 0.1405, 0.2886, 0.0397, 0.0148, 16.7235,
 122 (0804): 0.1793, 0.2115, 0.4135, 0.0752, 0.0240, 20.2183,
 138 (0820): 0.2276, 0.2949, 0.5513, 0.1272, 0.0358, 23.5304,
 154 (0836): 0.2761, 0.3888, 0.6983, 0.1981, 0.0500, 26.6725,
 170 (0852): 0.3231, 0.4896, 0.8485, 0.2877, 0.0662, 29.5960,
 186 (0908): 0.3332, 0.5395, 0.9058, 0.3585, 0.0763, 29.0546,
 202 (0924): 0.3713, 0.6359, 1.0380, 0.4698, 0.0936, 31.3031,
 218 (0940): 0.4059, 0.7297, 1.1619, 0.5909, 0.1112, 33.3339,
 234 (0956): 0.4365, 0.8178, 1.2743, 0.7169, 0.1285, 35.1402,
 250 (1012): 0.4646, 0.9021, 1.3791, 0.8469, 0.1456, 36.8123,
 266 (1028): 0.4887, 0.9785, 1.4713, 0.9745, 0.1617, 38.2516,
 282 (1044): 0.5024, 1.0343, 1.5324, 1.0837, 0.1744, 38.8181,
 298 (1100): 0.5145, 1.0831, 1.5850, 1.1853, 0.1859, 39.4437,
 314 (1116): 0.5261, 1.1278, 1.6331, 1.2806, 0.1965, 40.1370,
 330 (1132): 0.5419, 1.1818, 1.6954, 1.3849, 0.2086, 41.1018,
 346 (1148): 0.5569, 1.2309, 1.7522, 1.4807, 0.2196, 42.0990,
 362 (1204): 0.5525, 1.2352, 1.7467, 1.5179, 0.2224, 41.7398,
 378 (1220): 0.5594, 1.2631, 1.7769, 1.5786, 0.2290, 42.0942,
 394 (1236): 0.5649, 1.2847, 1.8003, 1.6260, 0.2342, 42.4019,
 410 (1252): 0.5687, 1.2996, 1.8162, 1.6588, 0.2377, 42.6257,
 426 (1308): 0.5706, 1.3073, 1.8244, 1.6764, 0.2396, 42.7414,
 442 (1324): 0.5705, 1.3077, 1.8246, 1.6783, 0.2398, 42.7324,
 458 (1340): 0.5684, 1.3008, 1.8166, 1.6644, 0.2382, 42.5887,
 474 (1356): 0.5642, 1.2866, 1.8003, 1.6349, 0.2349, 42.3064,
 490 (1412): 0.5579, 1.2651, 1.7760, 1.5902, 0.2299, 41.8873,
 506 (1428): 0.5495, 1.2365, 1.7437, 1.5313, 0.2233, 41.3382,
 522 (1444): 0.5392, 1.2012, 1.7036, 1.4590, 0.2152, 40.6711,
 538 (1500): 0.5271, 1.1593, 1.6561, 1.3748, 0.2057, 39.9030,
 554 (1516): 0.4360, 0.9453, 1.3621, 1.0888, 0.1657, 33.0141,
 570 (1532): 0.4231, 0.9000, 1.3102, 1.0013, 0.1555, 32.2590,
 586 (1548): 0.4105, 0.8545, 1.2589, 0.9127, 0.1452, 31.5636,
 602 (1604): 0.3987, 0.8091, 1.2084, 0.8240, 0.1349, 30.9761,
 618 (1620): 0.3872, 0.7617, 1.1562, 0.7340, 0.1242, 30.5381,
 634 (1636): 0.3692, 0.7021, 1.0851, 0.6343, 0.1116, 29.5661,
 650 (1652): 0.3461, 0.6335, 0.9993, 0.5313, 0.0978, 28.1805,
 666 (1708): 0.3186, 0.5570, 0.8996, 0.4284, 0.0832, 26.5533,
 682 (1724): 0.2884, 0.4782, 0.7933, 0.3328, 0.0688, 24.7675,
 698 (1740): 0.2557, 0.3987, 0.6819, 0.2472, 0.0550, 22.8149,
 714 (1756): 0.2206, 0.3204, 0.5671, 0.1737, 0.0421, 20.6839,
 730 (1812): 0.2454, 0.3387, 0.6233, 0.1570, 0.0421, 21.7836,
 746 (1828): 0.1940, 0.2437, 0.4685, 0.0942, 0.0285, 18.7687;
ENDX;
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June 28, 1985

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("NO2")
("HCHOr")
("HCHOs")
("O3toO1D")
("CCHO ")
("O3=O(3P)")
LIGHT=6#
   0 (0603): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0001,
   9 (0612): 0.0001, 0.0001, 0.0001, 0.0001, 0.0001,  0.0230,
  25 (0628): 0.0002, 0.0001, 0.0002, 0.0001, 0.0001,  0.2902,
  41 (0644): 0.0022, 0.0014, 0.0039, 0.0001, 0.0001,  1.2902,
  57 (0700): 0.0092, 0.0063, 0.0158, 0.0006, 0.0005,  3.1686,
  73 (0716): 0.0267, 0.0206, 0.0484, 0.0031, 0.0018,  6.0441,
  89 (0732): 0.0567, 0.0505, 0.1117, 0.0106, 0.0048,  9.5380,
 105 (0748): 0.0975, 0.0999, 0.2081, 0.0276, 0.0104, 13.3165,
 121 (0804): 0.1459, 0.1689, 0.3334, 0.0591, 0.0191, 17.1049,
 137 (0820): 0.1981, 0.2550, 0.4798, 0.1089, 0.0308, 20.7680,
 153 (0836): 0.2519, 0.3554, 0.6410, 0.1801, 0.0456, 24.2557,
 169 (0852): 0.3051, 0.4658, 0.8091, 0.2731, 0.0629, 27.5118,
 185 (0908): 0.3020, 0.4889, 0.8216, 0.3249, 0.0691, 26.8898,
 201 (0924): 0.3429, 0.5887, 0.9612, 0.4360, 0.0867, 29.3356,
 217 (0940): 0.3804, 0.6869, 1.0933, 0.5583, 0.1048, 31.5558,
 233 (0956): 0.4139, 0.7797, 1.2139, 0.6866, 0.1227, 33.5396,
 249 (1012): 0.4438, 0.8668, 1.3240, 0.8179, 0.1402, 35.3366,
 265 (1028): 0.4702, 0.9467, 1.4222, 0.9481, 0.1568, 36.9413,
 281 (1044): 0.4853, 1.0050, 1.4875, 1.0591, 0.1699, 37.5867,
 297 (1100): 0.4990, 1.0568, 1.5448, 1.1633, 0.1818, 38.3077,
 313 (1116): 0.5119, 1.1038, 1.5967, 1.2609, 0.1928, 39.0823,
 329 (1132): 0.5287, 1.1601, 1.6622, 1.3677, 0.2052, 40.1063,
 345 (1148): 0.5448, 1.2114, 1.7225, 1.4663, 0.2167, 41.1647,
 361 (1204): 0.5547, 1.2491, 1.7643, 1.5447, 0.2254, 41.6841,
 377 (1220): 0.5623, 1.2791, 1.7971, 1.6087, 0.2325, 42.0737,
 393 (1236): 0.5684, 1.3024, 1.8226, 1.6589, 0.2380, 42.4126,
 409 (1252): 0.5727, 1.3185, 1.8402, 1.6939, 0.2418, 42.6610,
 425 (1308): 0.3992, 0.9418, 1.3126, 1.2157, 0.1731, 27.0961,
 441 (1324): 0.3991, 0.9419, 1.3124, 1.2168, 0.1732, 27.0895,
 457 (1340): 0.3974, 0.9364, 1.3060, 1.2061, 0.1719, 26.9907,
 473 (1356): 0.3941, 0.9254, 1.2932, 1.1837, 0.1694, 26.7968,
 489 (1412): 0.3893, 0.9088, 1.2742, 1.1501, 0.1656, 26.5089,
 505 (1428): 0.3829, 0.8870, 1.2491, 1.1059, 0.1606, 26.1314,
 521 (1444): 0.3750, 0.8600, 1.2181, 1.0518, 0.1545, 25.6722,
 537 (1500): 0.3658, 0.8282, 1.1815, 0.9889, 0.1473, 25.1426,
 553 (1516): 0.4018, 0.8681, 1.2493, 1.0070, 0.1526, 31.5689,
 569 (1532): 0.3887, 0.8239, 1.1979, 0.9232, 0.1428, 30.7798,
 585 (1548): 0.3757, 0.7792, 1.1465, 0.8383, 0.1328, 30.0347,
 601 (1604): 0.3632, 0.7341, 1.0951, 0.7531, 0.1227, 29.3761,
 617 (1620): 0.3504, 0.6862, 1.0404, 0.6659, 0.1122, 28.8313,
 633 (1636): 0.3315, 0.6268, 0.9680, 0.5704, 0.0999, 27.7688,
 649 (1652): 0.3074, 0.5590, 0.8812, 0.4720, 0.0865, 26.2643,
 665 (1708): 0.2793, 0.4847, 0.7825, 0.3752, 0.0726, 24.5264,
 681 (1724): 0.2487, 0.4086, 0.6779, 0.2860, 0.0589, 22.6185,
 697 (1740): 0.2159, 0.3329, 0.5696, 0.2073, 0.0459, 20.5404,
 713 (1756): 0.1814, 0.2595, 0.4601, 0.1411, 0.0341, 18.2864,
 729 (1812): 0.1847, 0.2500, 0.4615, 0.1160, 0.0311, 17.8711,
 745 (1828): 0.1393, 0.1704, 0.3291, 0.0657, 0.0199, 14.9333;
ENDX;
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